PHD

The Integration of controllability into process design

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THE INTEGRATION OF CONTROLLABILITY

INTO

PROCESS DESIGN

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ABSTRACT

Rising costs of raw materials, increased competition and tighter environmental regulations have forced process designers to strive to obtain highly integrated designs which exhibit good dynamic behaviour. This, in turn, has necessitated the consideration of plant controllability at the design stage.

In this work, first, the plant characteristics which prevent the achievement of perfect control and limit the quality of control obtained from practical control systems are identified and treated in some detail. These are the nonminimum phase elements (time delays and right half plane zeros), saturation of the manipulated variables and plant sensitivity to modeling errors. A review of the recent attempts to develop controllability measures based on these plant characteristics is also given.

A multiobjective design algorithm which allows the simultaneous consideration of the economic and dynamic aspects is then proposed and applied to the design of an n-butane--isobutane spliter and a Continuous Stirred Tank Reactor (CSTR) in which a first order reaction takes place. The superiority of this design algorithm over the currently practiced design approach in which an economic performance index is optimised to yield the "best" design is clearly demonstrated by these two case studies.

Since the design of plant controllers is in itself a multiobjective problem, the proposed algorithm is also

applied to the design of Single Input Single Output (SISO) controllers. Again, the superiority of this technique over the currently available methods is demonstrated by the considered examples.

CONTENTS

CHAPTER 1

INTRODUCTION

During the last two decades the costs of raw materials have rapidly increased and competition has become tougher. These two facts have forced the process designers to strive for obtaining better designs than the existing overdesigned plants. This, in turn, has led to the appearance of highly integrated designs which contain a large number of recyle streams, few surge tanks and reduced equipment sizes. such new designs represent a relatively large reduction in the capital charges and the steady state operating costs which suggests that they are widely used in industry. The fact that this is not the case is usually due to their inherently poor dynamic characteristics and controllability.

The dynamic characteristics of a plant design are dictated by its structure and equipment sizes. This means that in order to ensure that a final design is operable and controllable the plant dynamics as well as its steady state economic aspects should be simulataneously considered at the different process design stages.

In this study we are interested in the design of fixed plant flowsheets and unit operations. At this stage, the current approach to obtaining the "best" design involves trading the fixed costs against the operating costs for various values of the design variables. The optimum design is the one yielding the minimum total costs. The actual behaviour of the process during operation, and in particular its controllability and operability, are only seriously considered once the steady state design is completed. As a result, the overall performance and economy of the operating plant could be disappointing due to the inherently poor dynamic characteristics associated with the particular design variables values of the final design. In this thesis, a design approach , which ensures that the best design is established, is proposed and applied to a number of case studies. The optimality of a plant is measured by a number of criteria which include the steady state costs as well as measures of its dynamic behaviour.

Before giving the outline of the thesis, it is appropriate at this point to mention two recent studies which have explicitly considered the plant dynamic aspects at the design stage. Both studies have addressed the problem of synthesising operable plant flowsheets. Lenhoff and Morari [1982] used a vector of two criteria and a bounding technique to evaluate and choose the best design from a carefully selected set of thermally coupled distillation columns designs. They employed the nominal vapour boilup as a measure of the economic performance of the process -- The capital charges were assumed to be negligible -- and a function of the controlled and manipulated variables deviations as a measure of its overall dynamic performance. The difficulty in choosing the weighting factors suggests that such a function should not be heavily relied on as a true measure of the plant controllability. Silverstein and Shinnar [1981] used frequency response arguments to analyse and study the controllability of a reactor with feed-effluent heat exchanger.

The structure of this thesis is as follows. Chapter 2 deals with process controllability, and the process characteristics which prevent the achievement of perfect control and limit the quality of control obtained from practical controller. In chapter 3 a new multiobjective approach to plant sizing is proposed. Some of the tools which have been used extensively in this investigation are briefly described in chapter 4. These are two continuous system simulation packages, ISIM and TUTSIM, and two direct search optimization methods, the "complex" method of Box [1965] and the Hooke and Jeeves [1961] method. In chapter 5, the proposed design algorithm is applied to the design of SISO controllers. Chapters 6 and 7 are, respectively, concerned with the integrated design and control of a CSTR and a binary distillation column. Chapter 8 presents a summary of the major conclusions drawn from this investigation. A few suggestions for further work are also given in this final chapter.

CHAPTER 2

PROCESS CONTROLLABILITY

2.1 Introduction

Troublesome control loops are not very uncommon in the processing industries. In most cases the bad performance of these loops is probably due to poorly designed and tuned controllers. However, there are instances where the uncontrollability of the process itself prevents the achievement of good control quality even if the best practical controller is used.

In the next section process controllability is defined and related concepts used in the control literature are briefly reviewed. The controller independent process characteristics which prevent the achievement of perfect control and limit the degree of process controllability are analysed, in detail, in section 2.4 after defining the process control objectives in section 2.3.

2.2 Process controllability

Basically, a process is said to be controllable if it can be controlled, through the use of a practical controller, and operated satisfactorily despite external and internal upsets. The ease by which the control objectives are achieved is referred to, in this thesis, as the degree of controllability. Many controllability criteria which are suitable for particular problems have appeared in the control literature. For completeness, a brief account of some of these definitions and their shortcomings is, here, given.

2.2.1 Complete state controllability

Consider the following time invariant system:

$$\dot{x}(t) = Ax(t) + Bu(t) \tag{2.1}$$

$$y(t) = Cx(t) \tag{2.2}$$

where $x(t)$ is an nx1 state vector, $u(t)$ is a rx1 input vector and $y(t)$ is a mx1 output vector. A, B, C are, respectively, nxn, nxr and mxn constant matrices.

This system is said to be completely state controllable if its state can be moved from a given initial state, $x(0)=x_1$, to the zero state, $x(t_1)=0$, within a finite time t_1, through the use of a piecewise continuous input vector, $u(t)$. It is well known that the necessary and sufficient condition for complete state controllability is that the matrix $[B,AB,A^2B,.....,A^{n-1}B]$ should have a rank equal to n. In some references, the term controllability when used on its own implies that some states but not all can be brought to the origin. Some of the shortcomings of this controllability definition are:

(a) Operational constraints may have to be violated as the paths followed by the different states in moving from their initial to final levels are not completely arbitrary.

(b) Manipulated variables constraints are not taken account of as it is assumed that unlimited control power is available.

(c) This definition is neither necessary nor sufficient for plant controllability and operability. Examples are given by Rosenbrock [1970].

2.2.2 Output controllability

This is an extention of the definition of state controllability which is concerned with the process outputs rather than the states. The system represented by equations (2.1) and (2.2) is said to be completely output controllable if and only if there exists a set of inputs which transfer any initial outputs, $y(0)=y_1$, to the zero outputs, $y(t_1)=0$, in a finite time t_1. Output controllability is garanteed if the rank of the matrix $[C, CAB, CA^2B, \ldots\ldots, CA^{n-1}B]$ is m. The shortcomings associated with the state controllability are also drawbacks of the output controllability definition.

2.2.3 Structural controllability

This concept, first introduced by Lin [1974], is aimed at pointing out whether a state uncontrollability of a plant is caused by the equipment designs and operating level or the structure of the plant/control system.

A pair [A,B] is structurally controllable if and only if there exists another pair $[A_0,B_0]$ of the same structure which is completely state controllable. Where the pair [A,B] denotes equation (2.1).

The existence of this second pair $[A_0,B_0]$ is assured if and only if (Shields and Pearson [1976]) :

(a) Every node is accessible from at least one control node. Where each input variable and each output variable is represented by a node.

(b) The generic rank of the compound matrix [A,B] is n. The first n columns of [A,B] are the columns of A and the rest are the columns of B. The generic rank is defined as the maximum rank a matrix can achieve.

2.2.4 Functional controllability

Here one is not concerned with the ability to transfer the system states or outputs from an initial to a final level but rather with the ability to force the process outputs to follow desired trajectories.

A linear time invariant system is said to be functionally controllable if, theoretically, there exists an input vector, u(t), defined for t>0 which generates any desired output trajectories, y(t), also defined for t>0.

Writting the system described by equations (2.1) and (2.2) into its transfer function form, we have:

$$Y(s) = G(s)U(s) \qquad (2.3)$$

where,

$$G(s) = C(sI-A)^{-1}B \qquad (2.4)$$

Rosenbrock [1970] indicated that system (2.3) is functionally controllable if det[G(s)]$\neq$0, and hence the system transfer matrix is square and nonsingular so that the required inputs may be obtained from:

$$U(s) = G^{-1}(s)Y(s) \qquad (2.5)$$

The main drawback of this controllability criterion is that no information is given about the trajectories of the inputs. The system constraints may or may not be violated.

These controllability criteria (state controllability, output controllability, functional controllability, etc.) are not suitable for analysing the degree of controllability and operability of chemical processes. This is not to say that they are not useful and they are but convenient mathematical definitions. On the contrary, they are appropriate for different engineering applications. For instance, state controllabilty is used in optimal control theory and is useful in process start-up and shut-down where the designer is interested in moving the plant from a given state to another. The structural controllabilty criterion is used in configuring and designing control structures, Johnston et al. [1985].

2.3 Control Objectives

Process controllers are judged according to the following criteria.

Disturbance rejection

The controlled variables should be kept at their desired values despite measured and unmeasured disturbances entering the system. Ideally one would like to achieve perfect control but, of course, in a real world this is unatainable. Attributes of the system closed loop response are used to measure the closeness of the control quality to this unachievable goal. A number of indices are used of which the maximum output deviation and the response settling time are two examples.

Servo control

Set points should be tracked fast and smoothly. The settling time, rise time and overshoot are the criteria by which the optimality of such behaviour is measured.

Overall performance indices such as the quarter decay ratio and weighted functions of the integral of the error are also frequently used to measure the quality of servo and regulatory control.

Robustness

Closed loop stability and performance should be maintained in the face of structural and parametric changes. Another important requirement is that the control system stability should be maintained in the case of an instrument failure. This is referred to as process integrity and it is treated as the next requirement from a process controller.

Integrity

Three types of possible instrument failures can occur in a control system, namely error detectors (monitors), actuators and measuring devices (transducers) failures. When any of these devices ceases to perform its task, the transient behaviour of the system may deteriorate to unacceptable levels or it may even be driven to instability. For Multiple Input Multiple Output (MIMO) systems when stability is preserved in spite of such occurances, the system is referred to as being of high integrity, Belletrutti and McFarlane [1971]. To allow for system integrity and the crippled system satisfactory behaviour, high performance of the normally operating control system is sacrificed by detuning the controllers. Such remedies are not always possible. There are two other possible ways of allowing for such difficulties. One approach is to install standby controllers in the positions where instrument failures may lead to highly unsatisfactory performance or instability of the operating plant. Cost and other difficulties such as those associated with bringing the standby controllers into smooth operation may rule out such a solution. Another possibility would be to allow for system integrity and anticipated difficulties at the process design stage.

Not too excessive control actions

High control actions increase the likelihood of manipulated variable saturation which in turn results in a considerable deterioration of the obtained control quality.

Controller transparency

A vital requirement is that the controller and the effects of the tuning parameters should be transparent to the operator. This is one of the main reasons why most of the modern approaches to controller design have found little success in industry.

Other desirable controller qualities may be found in the literature but they are, here, considered to be implied by the ones given above or are of minor importance.

2.4 Controller Independent Process Characteristics Which Limit the Achievable Quality of Control

Section 2.3 dealt with the desirable performance of a controlled process. These qualities are limited by the controller used as well as the process itself. Knowledge of the process features which limit the performance of any compensator help boost the confidence of the plant and control system designers in their decision making process. In this section, these difficult elements are identified and a review of the recent attempts to develop controllability measures based on these plant characteristics is given.

Consider the block diagram of the multivariable control system shown in figure 2.1. Where $P(s)$, $G(s)$ and $H(s)$ are transfer function matrices corresponding to the controller, plant and known disturbances respectively, whose elements are functions of the complex variable s. Their respective dimensions are (rxm), (mxr) and (mxk). $R(s)$, $E(s)$, $U(s)$, $Y(s)$ and $V(s)$ are, respectively, the (mx1) reference input transforms, (mx1) error transforms, (rx1) plant input transforms, (mx1) plant output transforms and (kx1) disturbance transforms.

The process outputs are given as:

$$Y = (I+GP)^{-1}GPR + (I+GP)^{-1}HV \tag{2.6}$$

and the controller outputs as:

$$U = (I+PG)^{-1}P(R-HV) \tag{2.7}$$

where I is an identity matrix of appropriate dimensions. For convenience the Laplace transform variable, s, is dropped. Assuming first that the system is closed loop stable, then for very "large" P which is equivalent to letting the controller gain of a Single Input Single Output (SISO) system tends towards infinity, the following result:

$$(I+PG)^{-1}P \simeq G^{-1} \tag{2.8}$$

$$(I+GP)^{-1}GP \simeq I \tag{2.9}$$

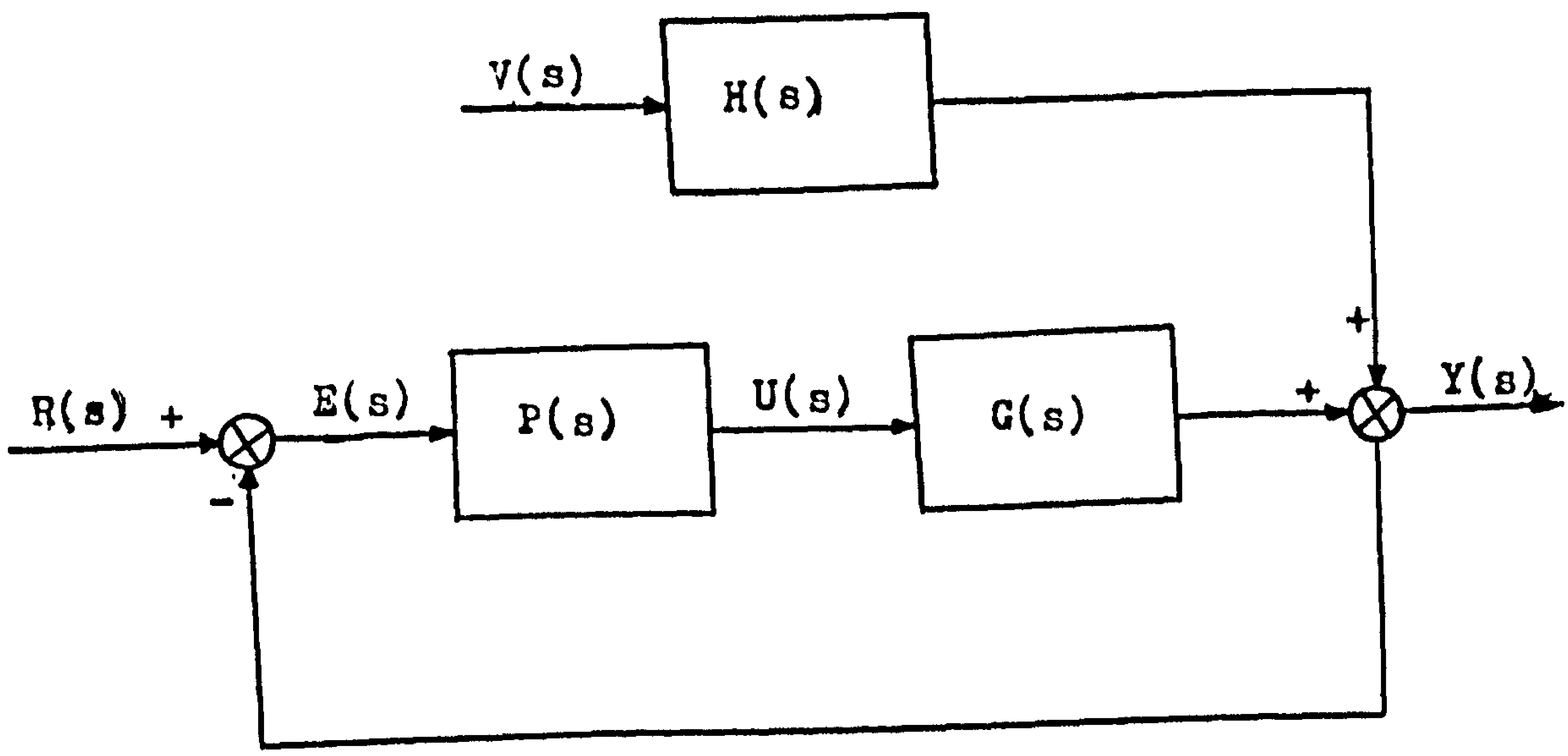


Figure 2.1 Block diagram of a multivariable control system

$$(I+GP)^{-1} \simeq 0 \tag{2.10}$$

Combining equations (2.6), (2.9) and (2.10) we have:

$$Y = R \quad \text{(perfect control)} \tag{2.11}$$

Relationships (2.8) and (2.7) yield:

$$U = G^{-1}(R-HV) \tag{2.12}$$

From equations (2.11) and (2.12) it is clear that for perfect control to be achieved, the plant transfer function matrix, G, should be invertible and that the inverse is implementable. For the inverse to exist, the process transfer function matrix must be square and hence the number of manipulated variables should be at least equal to the number of controlled variables. In the remainder of this chapter the plant transfer function matrix G(s) is assumed to be square with dimensions m. The process characteristics which prevent the implementation of the inverse are:

(a) Time delays:

The inverse is non-causal (contains predictive elements) if time delays are present in the elements of G.

(b) Right Half Plane (RHP) zeros:

The zeros of a transfer function matrix are the poles of its inverse and hence a plant transfer matrix which contains RHP zeros yields an unstable inverse.

(c) Manipulated variable saturation:

Saturation of the manipulated variables prevents the generation of the process input trajectories required for the achievement of good control.

(d) Plant/model mismatch:

The inverse can not be obtained if the true plant transfer function matrix is not known exactly.

These control quality limiting plant characteristics were also arrived at by Morari [1983] who used a new controller design framework, figure 2.2a, referred to as Internal Model Control (IMC) by Garcia and Morari [1982] and Inferential Control (IC) by Brosilow [1979]. In figure 2.2, G_m and G_c are, respectively, the plant model and controller transfer function matrices. D is the vector of unknown disturbances. The other variables are as defined earlier.

For a perfect plant model, $G_m = G$, the IMC structure reduces to that shown in figure 2.2b which is open loop control. The plant outputs are given by:

$$Y = GG_c(R-D) + D \tag{2.13}$$

Perfect control , Y=R, is achieved if the inverse of the

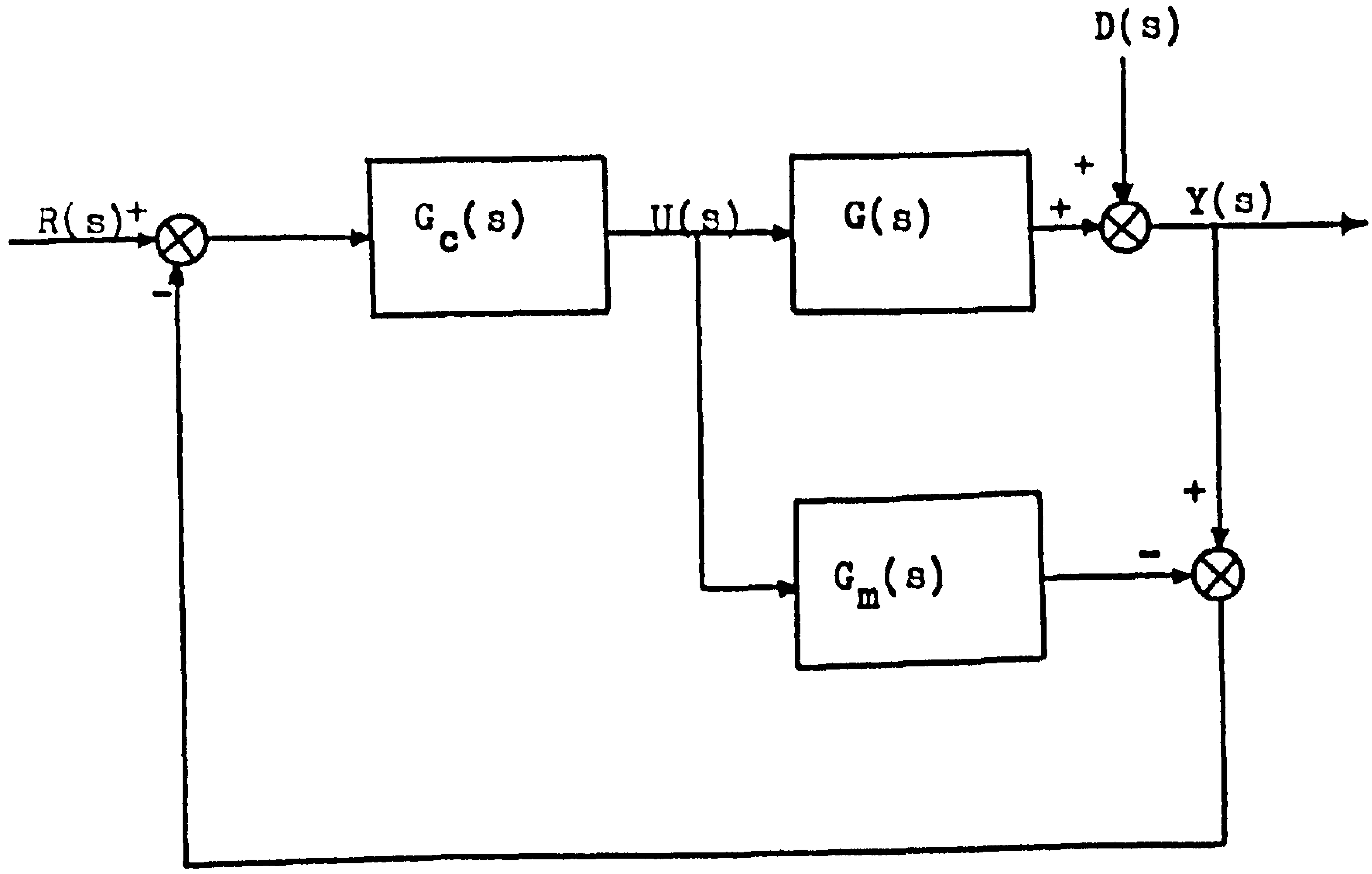


Figure 2.2a IMC structure

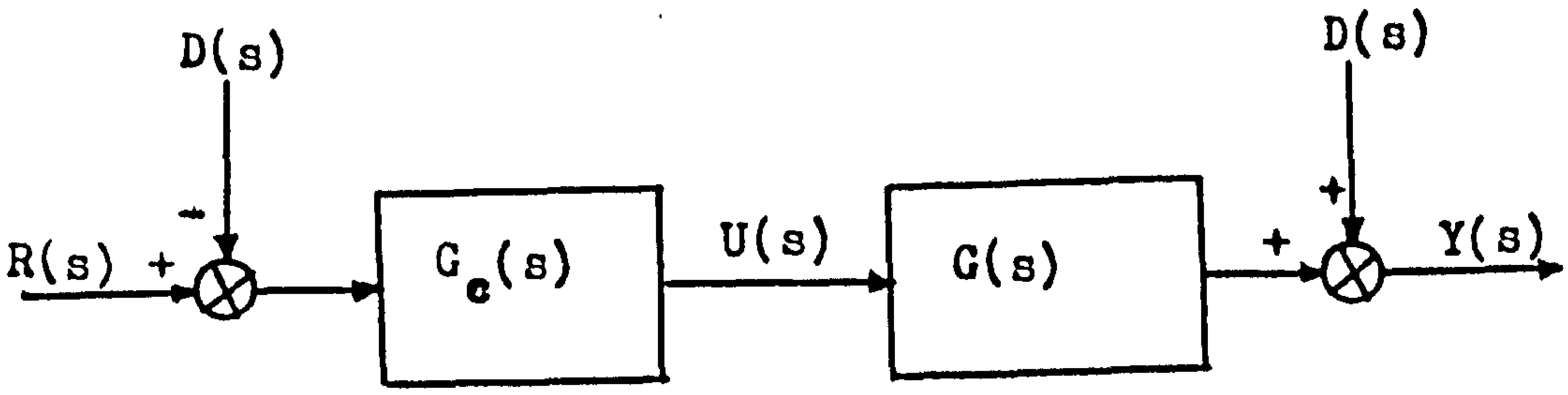


Figure 2.2b IMC structure for a perfect process model, $G_m(s)=G(s)$

plant transfer function matrix is used as the controller, i.e $G_c = G^{-1}$, and hence, again, perfect control is possible only if the plant matrix is invertible and its inverse is implementable.

The IMC structure and the conventional structure, figure 2.1, are equivalent if one of the two relationships holds:

$$G_c = P(I+G_m P)^{-1} \tag{2.14}$$

$$P = G_c(I-G_m G_c)^{-1} \tag{2.15}$$

2.4.1 Time delays

A common characteristic of most processes in the chemical and petrochemical industries is that, usually, when their inputs are changed, a finite time elapses before the outputs begin to change. Such a dynamic element is referred to as time delay, dead time, transportation lag or distance-velocity lag in fluid flow. The detrimental effects of time delays on system stability and control performance are well known. In frequency terms, the presence of dead times in the control loop contributes an additional phase lag which tends to destabilise the system.

Example 2.1: Effect of dead time on closed loop performance

Consider the SISO control loop system shown in figure 2.3. A First Order Plus Dead Time (FOPDT) plant is controlled using a Proportional plus Integral (PI) compensator. Where the plant time delay to time constant, ratio, T_d/T_c, is chosen to be either 0.5 or 1.0. Figures 2.4 and 2.5 give the system responses to unit step changes in the disturbance, $d_s(t)$, and the set point, $r_s(t)$, respectively. Subscript s is used to denote a scalar variable. Curves A and B refer to the smaller (0.5) and larger (1.0) dead time to time constant ratios respectively. For a step change in the set point the controller parameters have been calculated using the minimum IAE relationships of Rovira et al. [1969] and for a step change in the disturbance Lopez et al. [1967] minimum IAE relationships have been employed. For either set point or load disturbance changes it is quite apparent that large time delays have a detrimental effect on the control quality when conventional controllers are used.

The difficulty of controlling processes containing significant time delays have been the concern of the control engineering community for a long time and will continue to do so. This has led to the publication of a wealth of material on the topic. As a result new algorithms particularly suited for time delay compensation have been developed. By far, the most popular technique is the SISO Smith Linear Predictor (SLP) which was proposed by O. J. Smith [1957]. The method compensates for dead time by introducing a minor feedback loop around a conventional

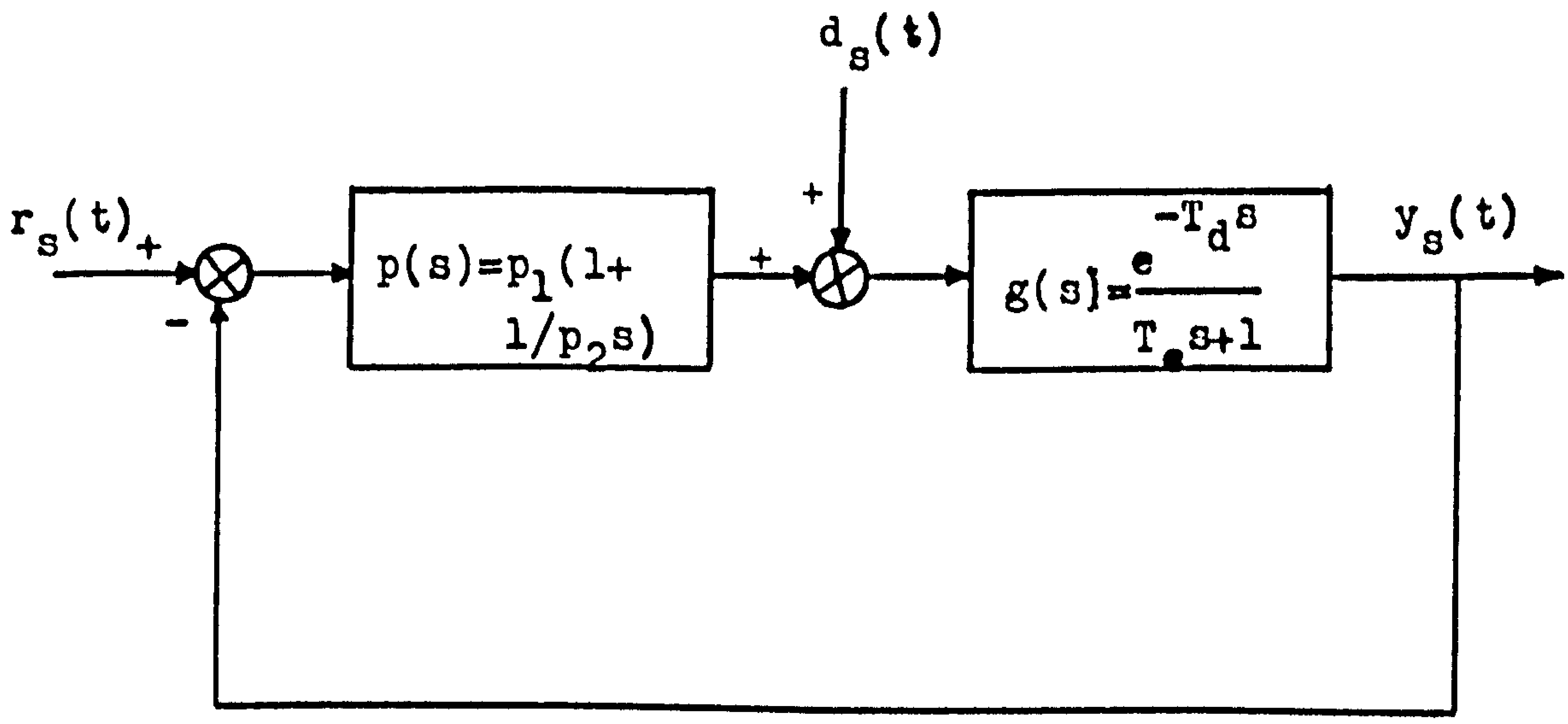


Figure 2.3 A SISO control system, $T_c=1$

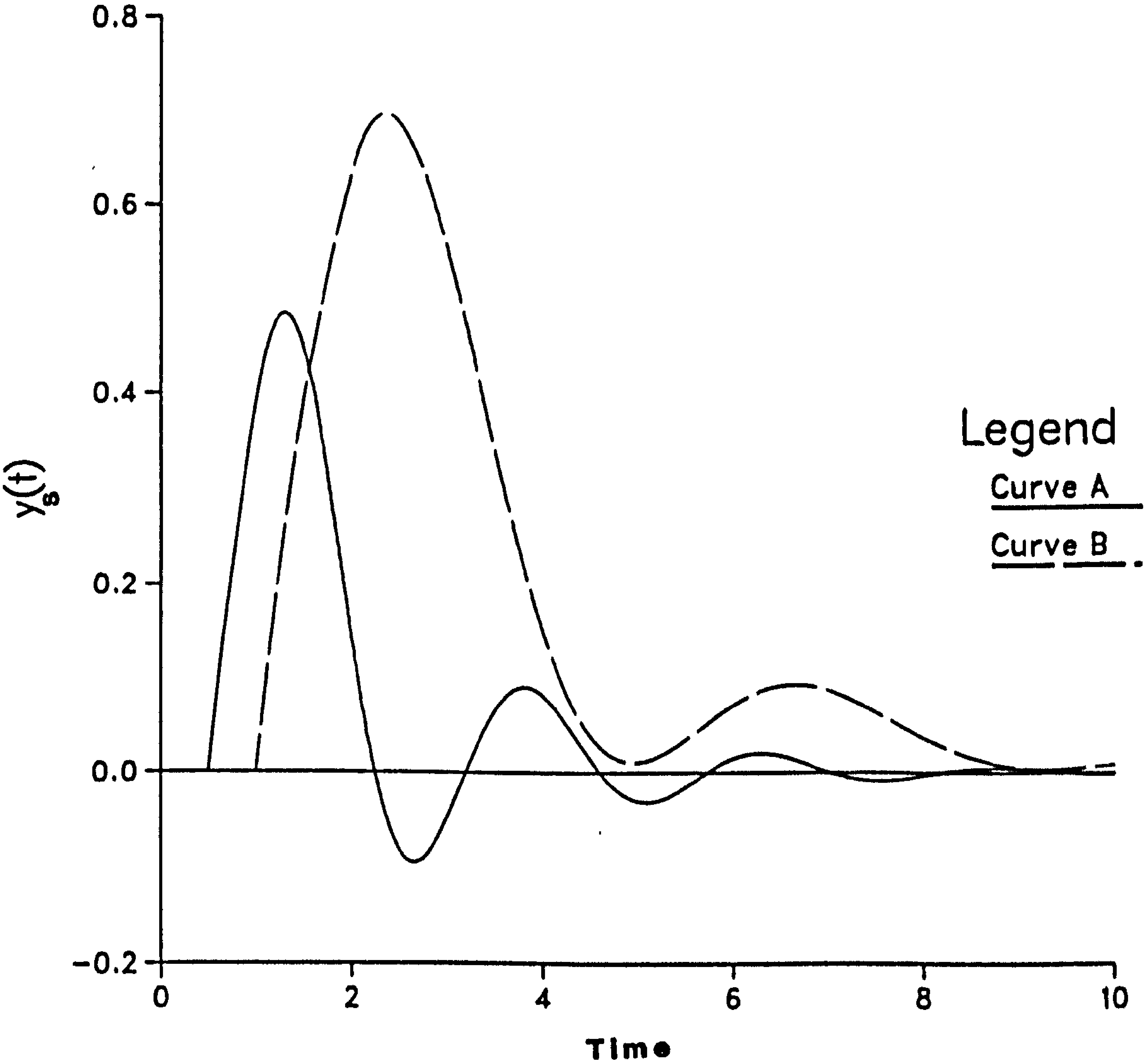


Figure 2.4 Response to a unit step change in the disturbance

Curve A --- T_d=0.5

Curve B --- T_d=1.0

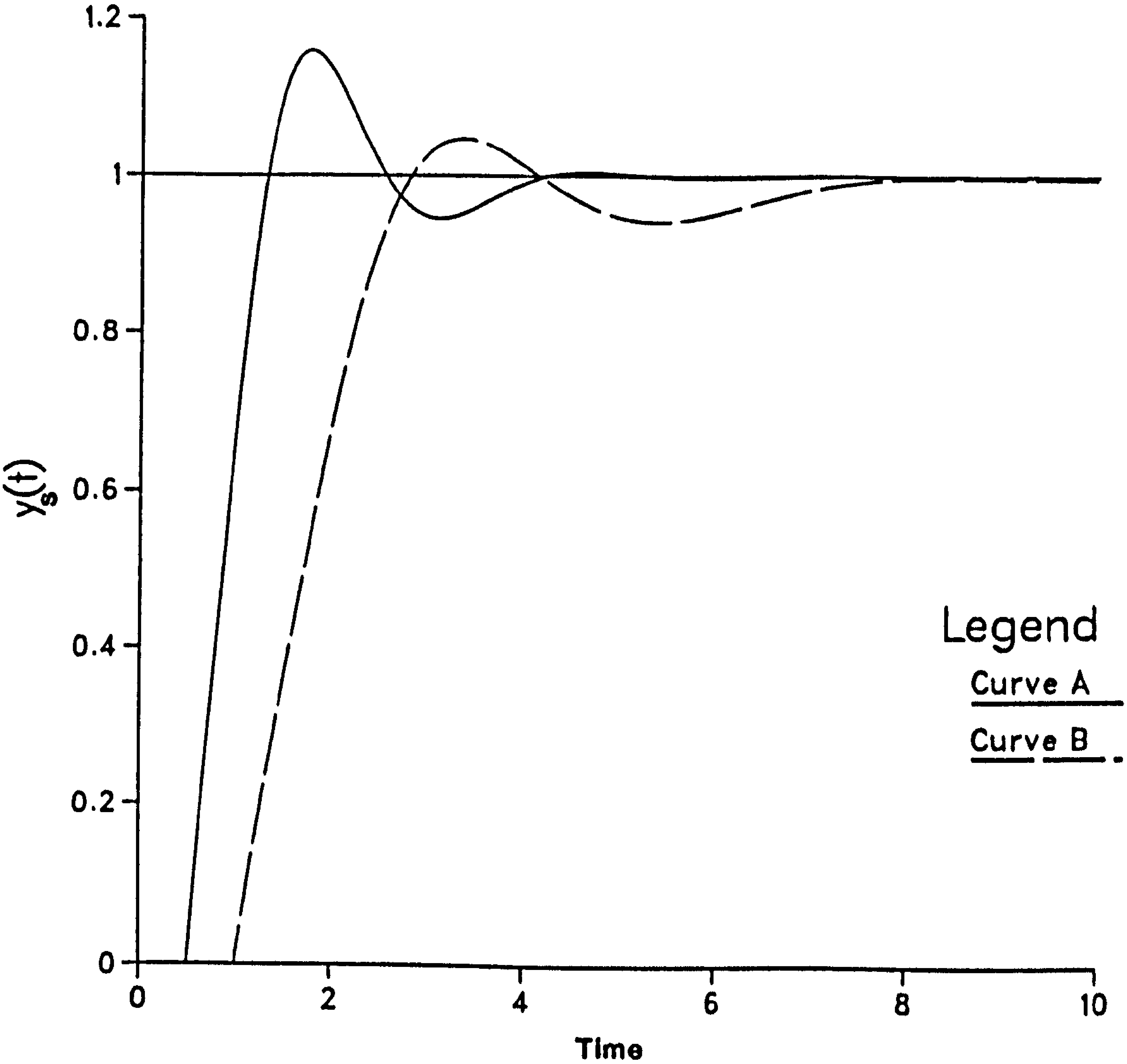


Figure 2.5 Response to a unit step change in the set point.

Curve A --- T_d=0.5

Curve B --- T_d=1.0

controller, figure 2.6a. Where subscript m refers to model. The output of the predictor block represents the difference between two responses: The response of a delay-free model of the process minus the response of the delayed model. For a perfect plant model, $g_m(s)=g(s)$, block manipulation reduces the original SLP scheme to that of figure 2.6b. This latter figure shows that the SLP removes the dead time from the feedback path and hence allows the controller to be designed for a delay-free system. Comparison of the performance of the SLP scheme with conventional PI and PID controllers can be found in the dissertation by Abbas [1982]. For more information on the SLP and other time delay compensation schemes the interested reader should consult the book by Marshall [1979] and the survey paper by Donoghue [1976].

Recently attempts have been made at developing quantitative measures for the assessment of the degree of controllability of time delay systems, Holt and Morari [1985b], and Perkins and Wong [1985].

In their approach, Holt and Morari [1985b] used the framework of IMC. For a perfect plant model, the plant outputs are given by equation (2.13) which is, for clarity, rewritten below:

$$Y = GG_c(R-D) + D \qquad (2.13)$$

Perfect control is achieved if the inverse of the plant

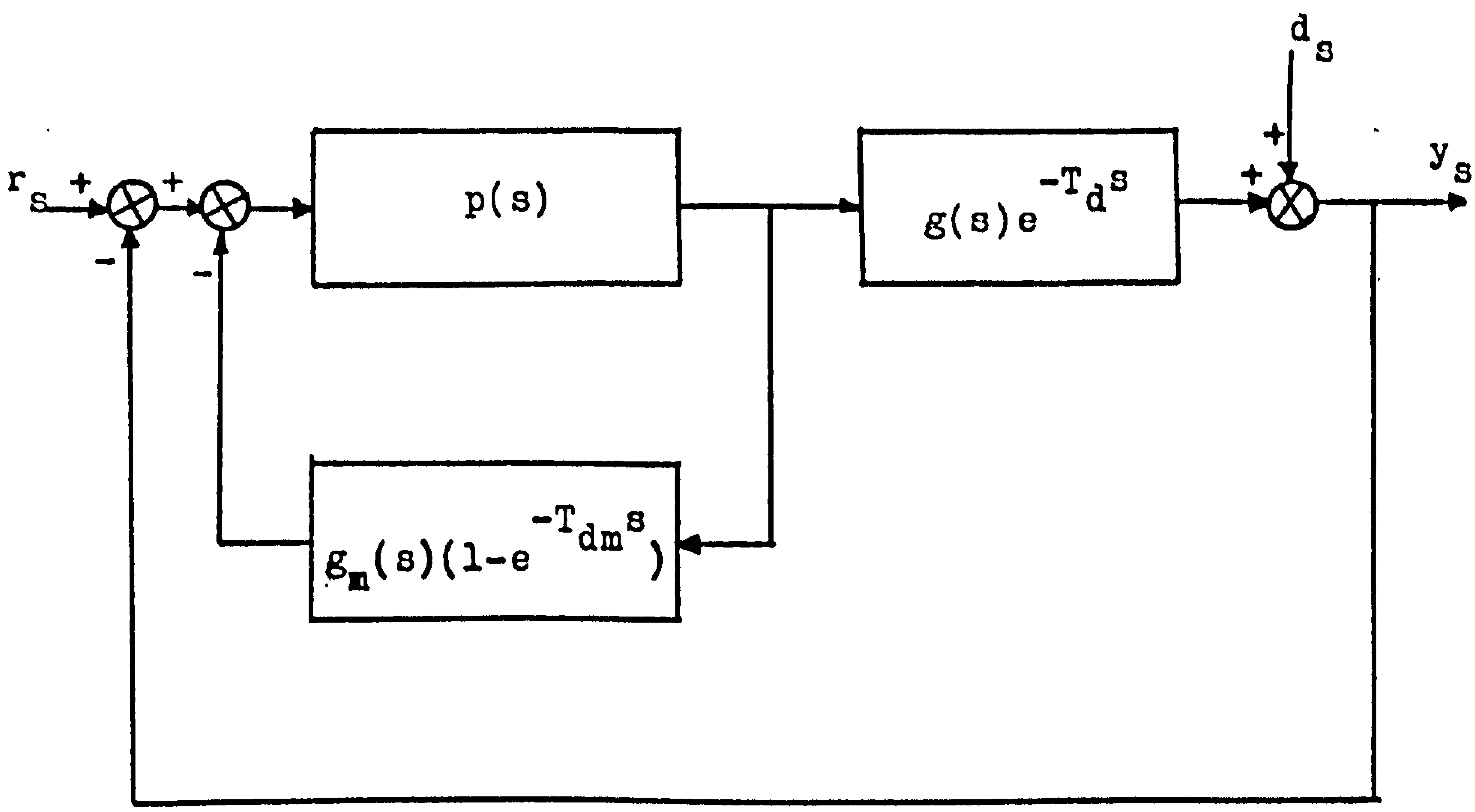


Figure 2.6a SLP scheme

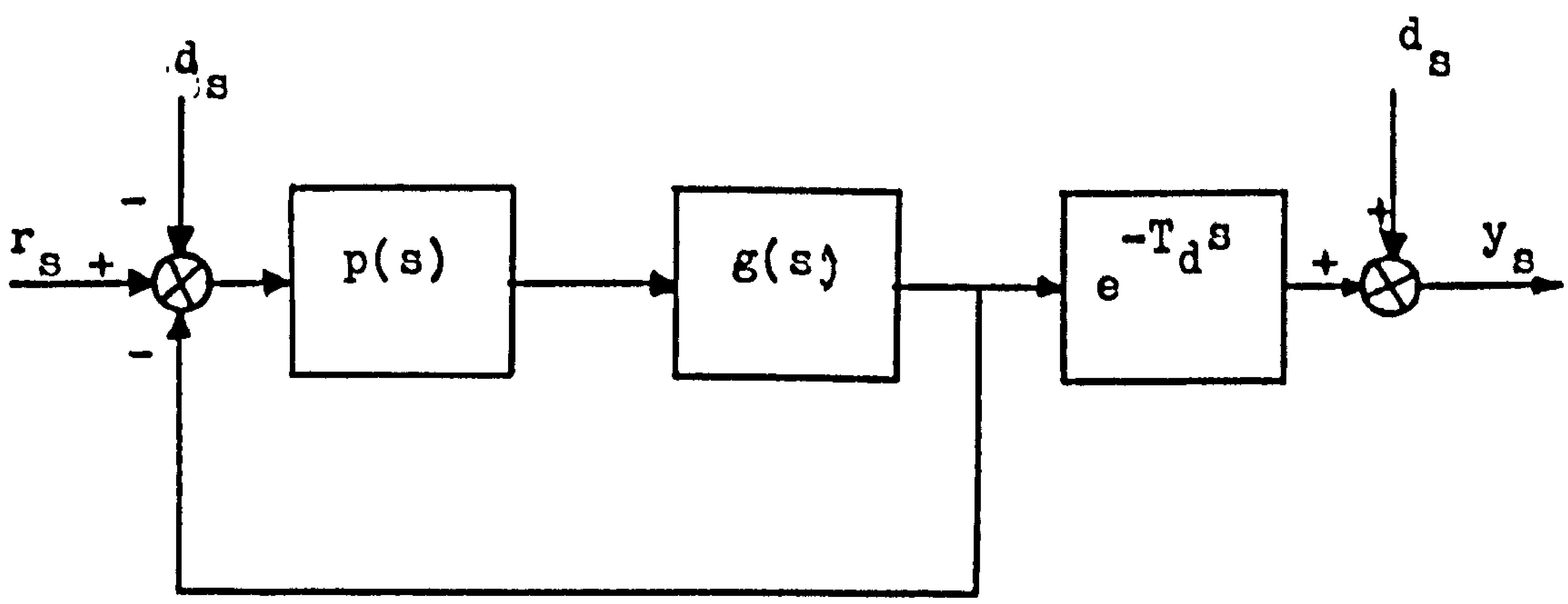


Figure 2.6b SLP for a perfect plant model,
i.e $g_m(s)=g(s)$ and $T_{dm}=T_d$

transfer function matrix is used as the controller, i.e $G_c = G^{-1}$. For a plant which exhibits dead times in its behaviour, the inverse can not be used as the controller because it contains predictive elements. To obtain a realisable compensator, the authors suggested that the plant transfer function matrix should be factored as:

$$G = G_+ G_- \qquad (2.16)$$

such that G_-^{-1}, which is used as the controller, is nonpredictive. Combining equations (2.13) and (2.16), we obtain:

$$Y = G_+(R-D) + D \qquad (2.17)$$

G_+ can be thought of as the closed loop transfer function matrix. As G_+ is the factor which prevents the achievement of perfect control, the authors proposed that it should be used as a measure of the difficulty of control introduced by the presence of time delays. For SISO systems the above factorisation is straightforward and it yields the result which has been known for a long time, namely the higher the process time delay the poorer the control system performance. For MIMO systems the factorisation is not unique, The reader is referred to the work of Holt and Morari [1985b] for an account of the difficulties involved and the analysis performed to arrive at the two measures they proposed for the evaluation of MIMO time delay systems. Here these two indices are stated without proof. The first measure is a lower bound on the minimum response time for the outputs:

$$G^* = \mathrm{diag}(s_i) \quad i=1,2, \ldots,m \tag{2.18}$$

where,

$$s_i = \min_j(s_{ij}) \quad j=1,2,3, \ldots,m \tag{2.19}$$

s_{ij} is the minimum delay in the numerator of the ijth element of G. G^* may or may not be a valid choice for G_+ The second measure is the fastest response obtainable by any controller with dynamic decoupling. in this case G_+ is given as:

$$G_+ = \mathrm{diag}(o_{ii}) \qquad i=1,2,\ldots,m \tag{2.20}$$

where,

$$o_{jj} = \exp\{-s\{\max_i [\max[0,(\hat{q}_{ij}-\hat{p}_{ij})]]\}\} \tag{2.21}$$

$\hat{p}_{ij}$ is the minimum delay in the numerator of the ijth element of G^{-1} and $\hat{q}_{ij}$ is the minimum delay in the denominator of the ijth element of G^{-1}.

These two measures, though easy to compute, are difficult to use by the designer in deciding on the best design even if time delays are the only criteria by which designs are to be ordered.

Perkins and Wong [1985] in trying to eleviate this difficulty they proposed a single measure which is defined as the minimum time delay, T_d, which allows the realisation of nonpredictive input functions to generate the following outputs:

$$Y = e^{-T_d s} k/s \tag{2.22}$$

where k is an (mx1) vector with all elements being unity. Equations (2.5) and (2.22) give this nonpredictive input vector as:

$$U = G^{-1} e^{-T_d s} k/s \tag{2.23}$$

One of the main drawbacks of this definition is that not much importance is given to the distribution of the time delay elements in the plant transfer function matrix.

2.4.2 Right Half Plane (RHP) zeros

Though known to cause control difficulties, RHP zeros have not received as much attention as time delays did. This is due to the fact that they are not very common in the chemical processing industries systems. For SISO systems right half plane zeros are often referred to as "inverse response". This is one of their properties in which the plant might initially responds in the opposite direction to where it eventially ends up.

2.4.2.1 SISO systems

RHP zeros are defined as the roots of the numerator polynomial of the plant transfer function whose real parts are greater than zero. Their properties are:

(a) The number of direction changes of the plant open loop response to a step input is equal to the number of RHP zeros present in the transfer function. For a plant containing an even number of RHP zeros, the initial response is in the proper direction and for a plant containing an odd number of RHP zeros the initial response is in the wrong direction.

(b) They exhibit robustness to model perturbations, Bristol [1981]. Small changes in the transfer function parameters do not shift the zeros of the closed loop system by a great deal.

(c) They are invariant under feedback control. A parallel path is required if they are to be shifted.

(d) The smaller the zeros, the more difficulty they present to feedback control. This can be seen from figure 2.7 where it is shown that as the zero is decreased the inverse response behaviour is more pronouced. A first order Tayler expansion of the time delay also stress this point:

$$e^{-T_d s} = 1 - T_d s \qquad (2.24)$$

The zero is decreased as the time delay is

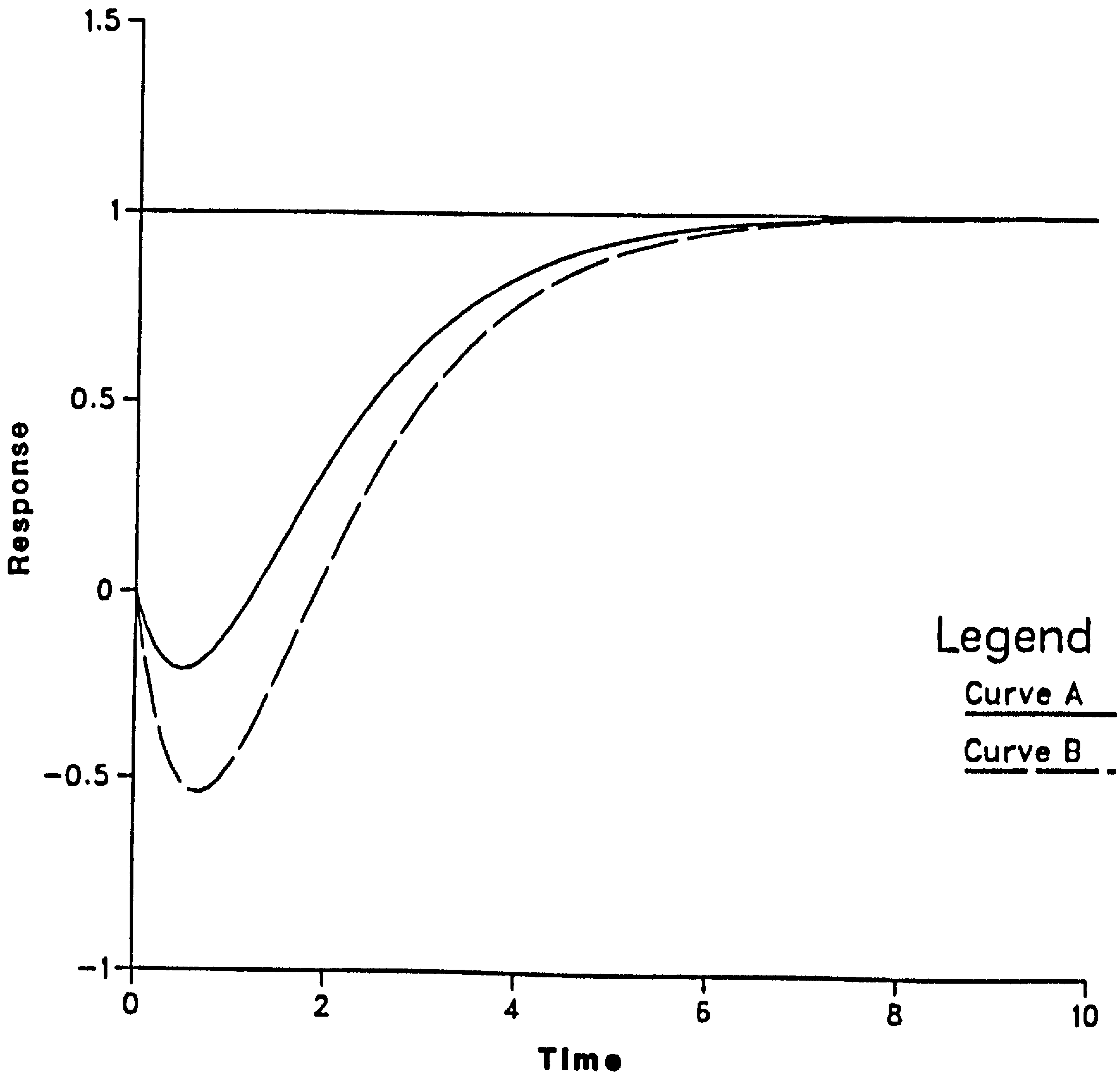


Figure 2.7 Unit step response of $\frac{(-zs+1)}{(s+1)(s+1)}$

Curve A --- z=1

Curve B --- z=2

increased.

(e) They become the unstable poles of the transfer function inverse.

Two examples in which RHP zeros have been reported to exist are distillation column base level and boiler drum level controls (Iinoya and Alpeter [1962], Shunta [1984], and Stephanopoulos [1984]).

Iinoya and Alpeter [1962] give a table of transfer functions and the conditions under which they give rise to RHP zeros. Based on the idea of the Smith Predictor, the authors have also suggested a compensator to deal with RHP zeros. The scheme serves to either remove the zeros or shift them to the Left Half Plane (LHP) with the latter approach being recommended. These ideas were later applied by Shunta [1984] to the two industrial examples cited above, i.e distillation and reboiler controls, and improvements over conventional controllers, PI in this case, were reported.

Again, using the IMC framework, Holt and Morari [1985a] suggested that the plant transfer function should be factored into two parts:

$$g = g_+ g_- \tag{2.25}$$

such that $|g_+|=1$. Where g_+ contains the RHP zeros. They have stated that if the minimum Integral of the Squared Error (ISE) is chosen as the performance index of the different plant designs then g_+ should be of the form:

$$g_+ = \frac{(-c_1 s+1)(-c_2 s+1)\ldots\ldots(-c_p s+1)}{(c_1 s+1)(c_2 s+1)\ldots\ldots(c_p s+1)} \qquad (2.26)$$

where $c_i=1/z_i$, z_i is the ith RHP zero and p is the number of RHP zeros of the plant. For a step input, the Minimum value of the ISE (MISE) is given by Frank [1974] as:

$$\text{MISE} = \sum_{i=1}^{p} \frac{2}{z_i} \qquad (2.27)$$

Holt and Morari [1985a] have shown that for the Integral of the Absolute Error the minimizing factorisation is given by:

$$g_+(s) = \prod_{i=1}^{p} \left(-\frac{1}{z_i}s + 1\right) \qquad (2.28)$$

and the Minimum value of the IAE (MIAE) is given by:

$$\text{MIAE} = \prod_{i=1}^{p} \frac{1}{z_i} \qquad (2.29)$$

Again, results (2.27) and (2.29) stress the point made earlier which states that small zeros are much more difficult to control than large ones.

2.4.2.2 MIMO Systems

The zeros and poles of a transfer function matrix are defined through its Smith-McMillan form:

$$M(s) = L(s)G(s)N(s) \qquad (2.30)$$

where L(s) and N(s) are unimodular matrices, i.e their respective determinants are constant.

$$M(s) = \mathrm{diag}(\phi_i(s)/\psi_i(s), 0) \quad i=1,2,\ldots,k \quad k \leq m \qquad (2.31)$$

where k is the rank of G(s).
The zeros of G(s) are defined to be the zeros of:

$$z(s) = \prod_{i=1}^{k} \phi_i(s) \qquad (2.32)$$

and its poles are defined to be the zeros of:

$$p(s) = \prod_{i=1}^{k} \psi_i(s) \qquad (2.33)$$

The zeros of G(s) which lie on the closed RHP plane are called RHP zeros or RHP Transmission (RHPT) zeros. They have the following properties.

(a) They are invariant under feedback control

(b) They become the unstable poles of the inverse.

Unlike the SISO case, no useful measures have been proposed for the quantification of the deterioration of control quality due to the presence of RHPT zeros. Wong [1985] suggested the use of a proportional feedback controller which has the form $P=p_1I$ -- I is the identity matrix -- as a measure of the difficulty of plant control caused by the presence of RHPT zeros. In particular, he suggested that the higher the value of the scalar gain p_1 required to destabilise the closed loop system, the better is the plant design. This result could be misleading as this proportional gain is dependent not only on the position of the RHP zeros in the complex plane but on the other plant steady state and dynamic characteristics as well.

2.4.3 Manipulated variables saturation

Apart from nonminimum phase (time delays and RHP zeros) elements, manipulated variables saturation is another limitation which leads to controller performance deterioration. For the achievement of perfect control the required input trajectories are given by equation (2.12) as:

$$U = G^{-1}(R-HV) \qquad (2.12)$$

Assuming that only disturbance inputs are anticipated we have:

$$U = WV \qquad (2.34)$$

where $W = -G^{-1}H$. W is here referred to as the disturbance matrix. From equation (2.34) it is apparent that the higher the disturbance gain, $\sigma/V = \dfrac{||U||_2}{||V||_2}$, the greater is the possibility for manipulated variables saturation. Where $||.||_2$ denotes the Eucledean vector norm (vector size) which is defined in equation (2.43) below. For SISO systems σ/V is simply the modulus of the scalar transfer function w(s) which is dependent on the frequency only. But for MIMO systems The gain is dependent on the direction of the disturbance vector , V, as well as the frequency. For any disturbance input, the multivariable gain , σ/V, is a linear function of principal gains (singular values) of the transfer function matrix W(s), MacFarlane and Scott-Jones [1979]. Also the following relationship holds:

$$\gamma_{min} \leqslant \sigma/V \leqslant \gamma_{max} \tag{2.35}$$

where γ_{min} and γ_{max} are the minimum and maximum singular values of the matrix W. Hence the lower the principal gains of the disturbance transfer function matrix, with particular emphasis on the maximum value, the better is the design.

The singular values of a matrix can be readily calculated using the SSVDC subroutine of the LINPACK package, Dongarra et al. [1979]. Alternatively the NAG library can be used since the principal gains of a matrix W are given as the square root of the eigenvalues of the matrix W^HW. Where superscript H denotes the conjugate transpose.

2.4.4 Plant/Model Mismatch

In the above analysis, the exact process model is assumed to be available. In practice this is never the case as assumptions are always introduced when plants are identified. Constant plant parameters and neglected dynamics are two examples. The inverse can not be obtained if the plant model is not known exactly. The control quality of a process will always differ from that of its model. For MIMO systems not only is this difference in performance a function of the magnitude of the plant/model mismatch but also the transfer function matrix condition, i.e plant sensitivity to modeling errors.

The open loop plant outputs are given by:

$$Y = GU \tag{2.36}$$

Suppose that small changes from G to G+ δG and Y to $Y+\delta Y$ produce a change in the input vector from U to $U+\delta U$, then:

$$(G+\delta G)(U+\delta U) = Y+\delta Y \tag{2.37}$$

Manipulation of equation (2.37), Noble [1969], yields:

$$\frac{||\delta U||}{||U||} \leqslant TK(G)\left[\frac{||\delta Y||}{||Y||} + \frac{||\delta G||}{||G||}\right] \tag{2.38}$$

where,

$$T = (1-||\delta G||.||G^{-1}||)^{-1} \tag{2.39}$$

and

$$K(G) = ||G||.||G^{-1}|| \tag{2.40}$$

$||.||$ denotes the norm and $K(G)$ is known as the condition number. For very small changes in G, it is apparent from equation (2.39) that T is approximately equal to one. Therefore, for changes in G only equation (2.38) reduces to:

$$\frac{||\delta U||}{||U||} < K(G)\left[\frac{||\delta G||}{||G||}\right] \tag{2.41}$$

Inequality (2.41) shows that if the condition number is small, a small change in the plant transfer function matrix yields a small change in the plant inputs. in such a case the transfer function matrix G(s) is said to be well conditioned. This has led Morari [1983] to propose the condition number of G(s) as a measure of the plant sensitivity to modeling errors. However, a drawback of the condition number is that it is dependent on the particular numerical values of the elements of G(s) (scale) and the norm definition used.

Three vector and matrix norms are commonly used in the field of numerical analysis. These are:

vector norms:

$$||a||_1 = \sum_{i}^{n} |a_i| \tag{2.42}$$

$$||a||_2 = \left[\sum_{i}^{n} |a_i|^2 \right]^{1/2} \tag{2.43}$$

$$||a||_\infty = \max_{i} |a_i| \tag{2.44}$$

matrix norms:

$$||X||_1 = \max_{j} \sum_{i}^{k} |x_{ij}| \tag{2.45}$$

$$||X||_2 = \max_{i} \lambda_i^{\frac{1}{2}}(X^H X) \tag{2.46}$$

$$||X||_\infty = \max_{i} \sum_{j}^{m} |x_{ij}| \tag{2.47}$$

where λ_i's are the eigenvalues of the matrix $(X^H X)$. a is an (nx1) vector and X is a (kxm) matrix . The ith norm of a vector or a matrix, $||.||_i$, is usually called the l_i -norm.

It has been suggested in the literature that using the optimum (minimum) condition number solves the problem of scaling. A review of the available approaches for scaling matrices to yield the minimum condition number is given by Wong [1985]. Apparently the optimum l_2 -norm is as yet a problem without a solution except for 2x2 matrices. Scaling matrices for minimum condition number of 2x2 matrices have been recently obtained by Grosdidier et al. [1985].

2.4.5 Discussion

Though the plant characteristics given above, i.e time delays, RHP zeros, Manipulated variables saturation and plant/model mismatch, prevent the achievement of perfect control and limit the control quality obtained from real systems, their effects differ from case to case and are dependent on the controller used. The following example serves to illustrate this point.

Example 2.2: Performance improvement through the use of a time delay and plant/model mismatch

It is desired to design a controller for a SISO plant, whose transfer function is given by:

$$g(s) = \frac{1}{s(2s+1)} \tag{2.48}$$

such that the ISE is minimized when a unit step input in the set point is applied. Choosing a Proportional controller with a gain p_1, figure 2.8a, and using Parseval's theorem the ISE is obtained as:

$$ISE = \frac{2p_1+1}{2p_1} \tag{2.49}$$

Suppose that for practical reasons the controller gain

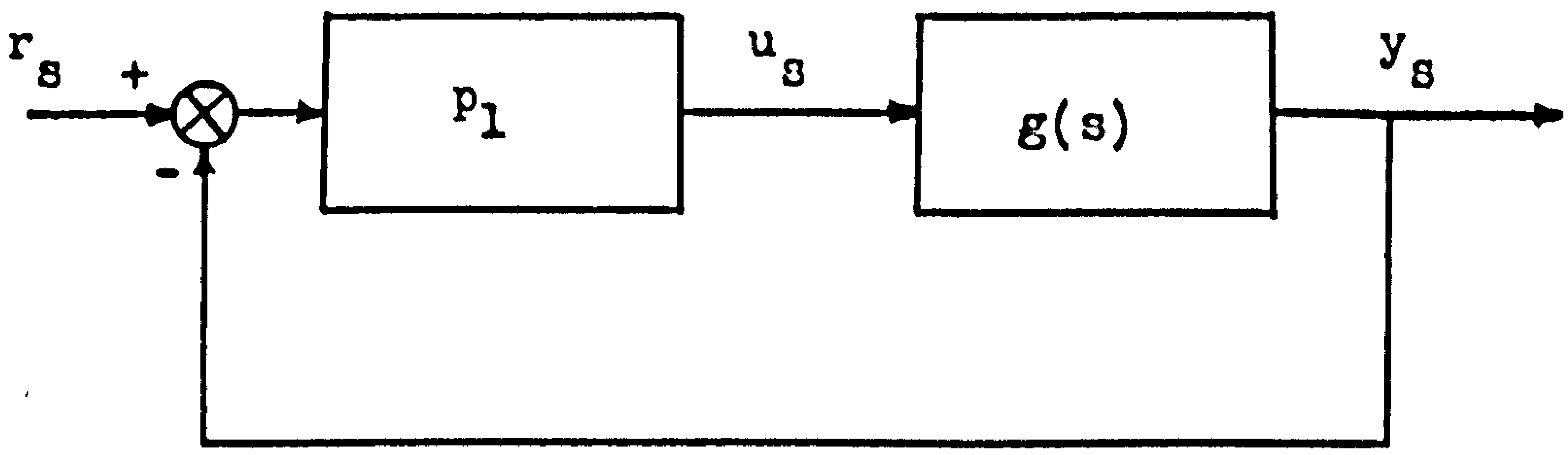


Figure 2.8a Delay-free system

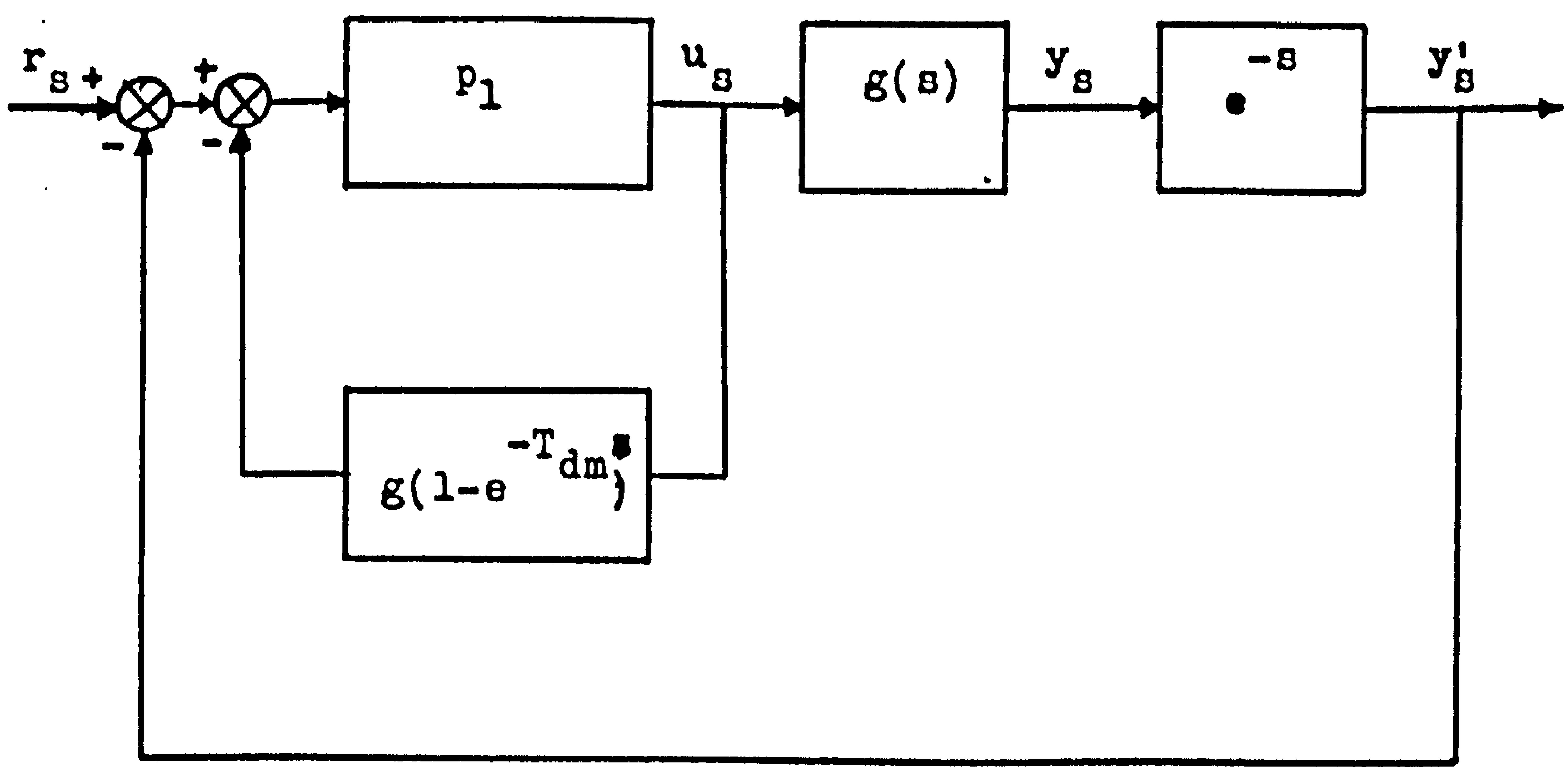


Figure 2.8b Modified system

is not to exceed a value of 0.5. Then the lowest possible value of the ISE which can be obtained is equal to 2.0. Adding an artificial time delay, $T_d=1$, to the plant transfer function and a Smith predictor loop to deal with this delayed plant, figure 2.8b, the same minimum ISE value, as the delay-free system is obtained, i.e 2. For calculation of the ISE the output of the original plant, $y_s(t)$, is used and not that of the delayed process, $y'_s(t)$. Varying the predictor time delay which is equivalent to the existence of a plant/model mismatch, the optimum ISE varies as shown in figure 2.9. An interesting result, here, is that contrary to the expected performance deterioration due to the presence of time delays and modeling errors, improvements in the quality of control may be obtained. As the predictor time delay is increased the minimum ISE value is reduced and it reaches its minimum value at +55% mismatch in the delay. A reduction of about 3% in the minimum ISE is achieved. The response of this system together with that obtained from the best delay free system are given in figure 2.10. From this figure it can be clearly seen that the use of time delays together with plant/model mismatch has improved the performance substantially. This is not a unique case. Other examples can be found elsewhere, Marshall et al [1982] and Abbas et al. [1986].

This example has clearly illusrated that, though time delays, RHPT zeros, manipulated variables saturation and modeling errors are process characteristics which generally

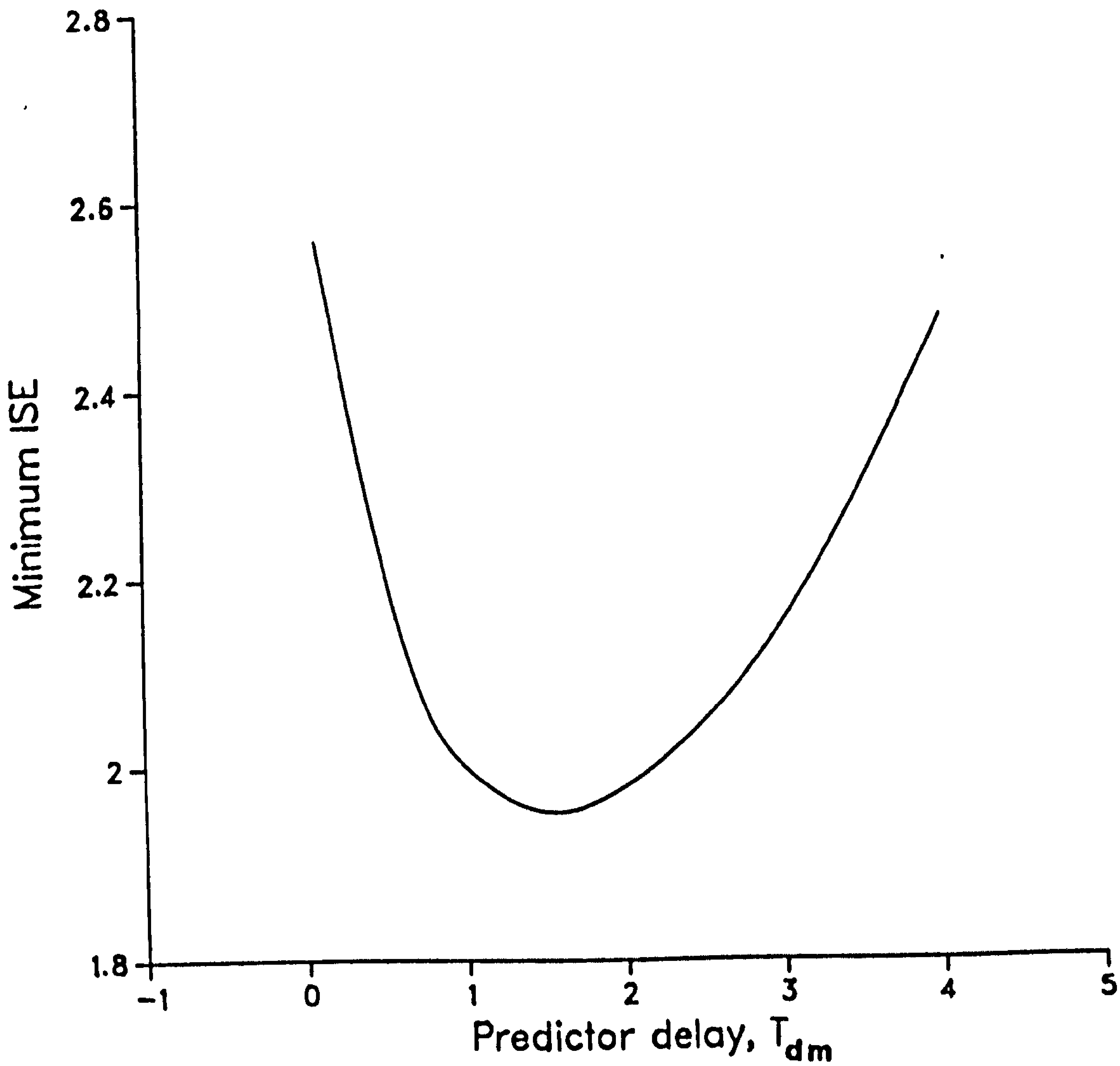


Figure 2.9 Variation of the minimum ISE with predictor delay, T_{dm}.

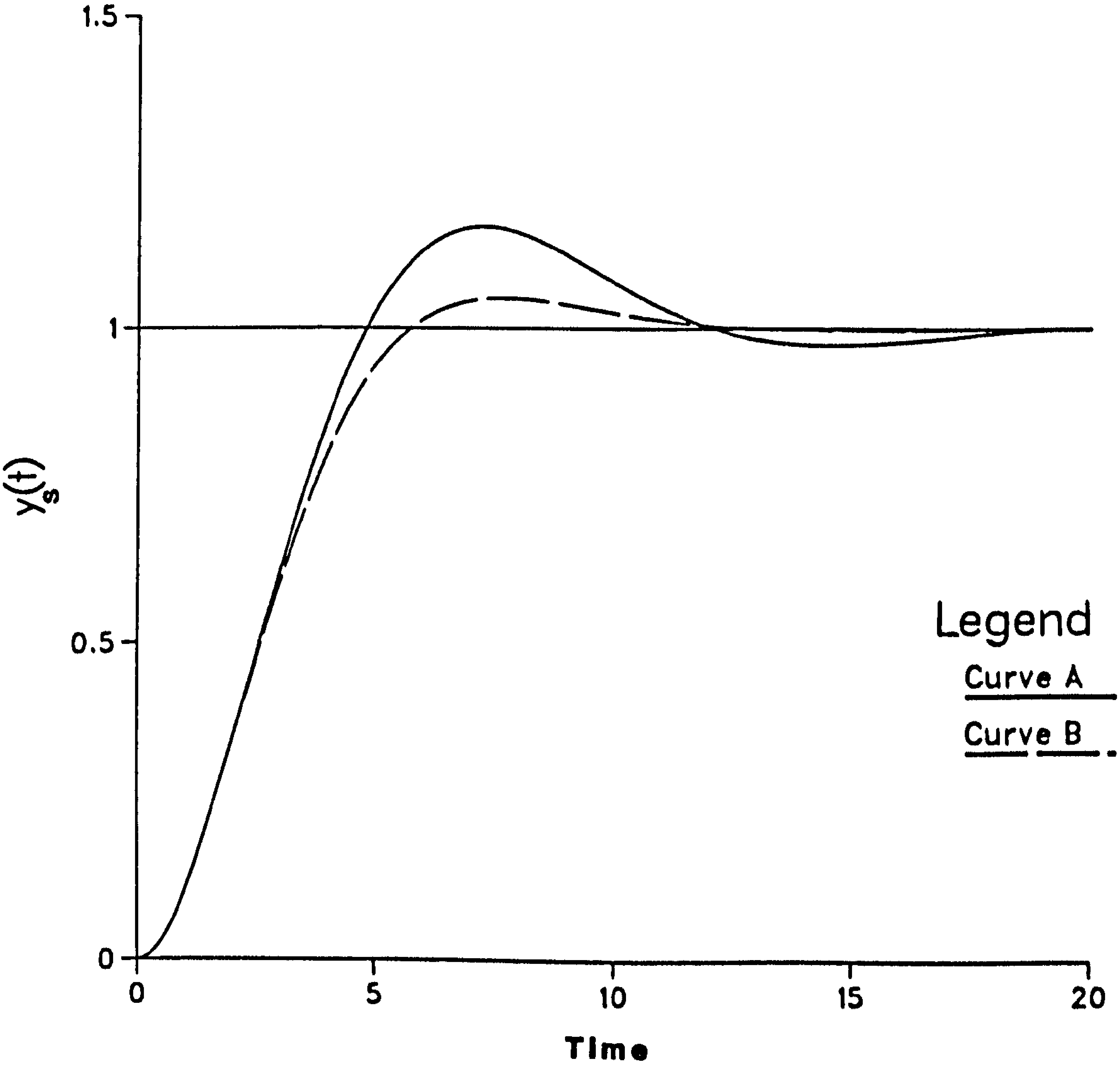


Figure 2.10 System response to a unit step change in the set point.
Curve A --- delay-free system
Curve B --- modified system.

limit the controller performance, the extent of performance deterioration is dependent on the compensators used. In addition, the difficulty of developing sound quantitative controllability measures based on these plant characteristics alone has been clearly illustrated by the attempts of Holt and Morari [1985a&b], and Perkins and Wong [1985]. This suggests that the indices proposed, if any, by these authors should only be used as guidelines at the early design stages before a plant structure is fixed.

CHAPTER 3

PROCESS DESIGN

3.1 Problem Statement

The design of a complete chemical plant involves the specification of the process route, the selection of the process flowsheet, the determination of the operating conditions and equipment sizes, and the choice of the control system. Normally, there exists a large number of feasible designs, and the designer task is to select the best controlled plant.

A rigorous approach to solving the problem is for the designer to form a meaningful overall performance index from the various design objectives which include capital and operating costs, controllability, flexibility, reliability and safety. Flexibility is concerned with the problem of ensuring feasible operation over a wide range of operating conditions, reliability is concerned with the probability of normal operation in the face of hardeware failures and safety is concerned with the hazards which might result from such failures. This performance index is then evaluated for every feasible plant. The optimum design is chosen as the alternative with the highest or lowest value of the performance index, depending on the problem formulation.

It is intuitively clear that such an approach is impractical and imfeasible. Two of the numerous reasons are:

(a) The designer is asked a priori to form an objective function from a vector of noncommensurable and nonquantifiable criteria. Even the most gifted designer, if faced with this situation, will not be able to formulate such a meaningful performance index.

(b) The number of feasible process alternatives (controlled plants) is extremely large and hence using presently available tools, the time taken to arrive, if ever, at the problem solution may be measured by years rather than minutes and hours.

The key to reducing the problem complexity and dimensionality is the introduction of assumptions and decomposition. In the currently practiced design method the plant is divided into smaller sections and the design of each section is decomposed into several activities which are performed more or less sequentially. An oversimplified outline of this design approach will serve to illustrate the difficulties which might arise in the final operating plant.

Process Synthesis

Here, the process route (chemical and physical transformations) and the process flowsheet (type of equipments and the interconnections between them) are fixed. This is the design stage where the decision maker's creativity, judgement and intuition are heavily tested. Although investement costs are his main concern, other criteria will definitely be included in his subjective judgement as he would, most probably, have experienced operational difficulties due to mal-structured sections of existing plants. There exist methods which help the designer synthesise good plant structures, and these are mainly time tested heuristic approaches. Algorithmic methods have also been developed and research is continuing in this direction, Stephanopoulos [1980].

Equipment Capacities and Operating Conditions Determination

At this design stage, a cost function is formulated. The feasible design which minimizes this function is considered to be the best solution. This design activity is treated in more detail in section 3.2.

Control System Synthesis

The synthesis of a control system involves the formulation of the control objectives and the selection of the measured variables, the manipulated variables, the control structure connecting the manipulations and the measurements as well as the control law between them.

For regulatory control, the task of connecting the measured and manipulated variables, and designing the control laws between them lends itself to rigorous theoretical analysis. This is demonstrated by the already large and growing number of available techniques. These are either frequency or time domain methods. Optimal control theory is an example. Another approach, used in industry, is to pair the measured and manipulated variables using the Relative Gain Array (RGA), Bristol [1966] and Shinskey [1967]. The resulting SISO controllers connecting the two sets of variables are then tuned using any of the available techniques such as the one proposed in chapter 5. Reviews of most of the available techniques for designing control systems for plants with fixed sets of manipulated and controlled variables are given by Ray [1983] and Edgar [1976]. However rules of thumb are heavily relied on in the selection of these manipulated and controlled variables. Some of these heuristics are given by Morari [1982] and Hougen et al [1969]. It is only recently that attempts have been made to systemise this extremely important activity of the control system synthesis phase. The interested reader is referred to the two papers by Johnston et al. [1983] and Stephanopoulos [1982] for comprehensive reviews of these attempts.

Choosing a process flowsheet structure fixes the most profitable, the safest and the most controllable designs which can be obtained. Since the steady state profit is more or less the sole criterion by which the sizes of the process units are determined, the maximum attainable levels of the other criteria are further restricted or fixed at the end of the second design phase. It is at this stage that this final plant design may exhibit highly undesirable dynamic behaviour such as unstability, long time delays and high interaction, and that it can not be adequately controlled even if the best control system is used. To allow for such difficulties, usually, large intermediate storage tanks are used to decouple the plant equipments and the units themselves are overdesigned. These overdesigns result in a considerable increase in capital costs and if not chosen properly, they may not improve the process dynamic behaviour and its degree of controllability. It has to be mentioned that that these overdesigns are intended for improving the process degree of flexibility as well but, again, contrary to one's intuition, such sought improvements may not be obtained, Grossman and Morari [1984].

In view of these shortcomings of the above outlined design method, approaches which introduce some integration such that explicit measures of the design objectives are considered simultaneously at the different design stages, are needed. Any proposed technique, however, should preserve the simplicity aspects of the method. In this work, we are interested in the simultaneous consideration of the process dynamics and degree of controllability together with the steady state costs in the design of fixed process flowsheet structures or unit operations. A design approach, based on the theory of Multiple Criteria Decision Analysis (MCDA), is proposed in section 3.2. Explicit allowance for other criteria such as flexibility and reliability have been recently considered by Swaney et al.

[1982] and Henley et al. [1981].

3.2 Integrated Process Design

3.2.1 Current approach to plant sizing

The normal approach to the design of a given process flowsheet structure is to define a cost function which includes the capital and operating charges, a statement of the desired production rate, a set of equations describing the operation of the processing units and a set of inequalities describing the physical operating limits or product specifications. Values of the design parameters which minimize the cost function subject to the plant equality and inequality constraints are taken as those values which yield the best design. Mathematically, this problem definition can be formulated as:

$$\min_{x} \{f_1(x):D\} \qquad (3.1)$$

where $D=\{g(x)\geqslant 0;h(x)=0\}$. x is the vector of design variables. $h(x)=0$ and $g(x)\geqslant 0$ are, respectively, the vector of the system state equations and the vector of inequalities. $f_1(x)$ is the total cost function.

Though it might appear to be a simple exercise, for many cases arriving at the solution of this nonlinear programming problem is no easy matter. Some of the difficulties which might be encountered at the problem formulation or solution stages are:

(a) Equipment costs and sales prices are often discontinuous and not known exactly.

(b) For complex units, some of the input-ouptut relationships are given by nonlinear ordinary or partial differential equations which often can not be solved to give explicit relationships.

(c) The lack of a single, highly reliable optimization algorithm which is suitable for most problems. This is underlined by the already high and growing number of available methods, Sargent [1980].

(d) It is assumed that a production rate is known. But in reality this is established through a detailed market analysis. Hence the given production rate is only a representation of the best engineering estimate available.

(e) System parameters like mass transfer coefficients, kinetic rate constants and physical properties are seldom known to a high degree of accuracy. The effects of these uncertainties on the final design might be considerable, and hence it has to be operated at a lower capacity than it was designed for. To allow for these uncertainties many researchers have reformulated the problem as a stochastic one by taking advantage of the available statistical approaches, Marketos [1975] and Halemane et al. [1983]. However, these approaches have many shortcomings as pointed out by Morari [1982].

A major drawback of this design technique is that the best design is chosen on the basis of the steady state costs alone. An operating plant is never at steady state as it is continuously bombarded by internal and external disturbances. This suggests that in obtaining the best design a number of criteria which include the steady state costs as well as a set of dynamic measures should be minimized. However, usually these criteria are in conflict and can not be simultaneously optimised. This means that the set of feasible designs can not be completely ordered. Partial odering is, However, possible and this has been the subject of the recently revived theory known as Multiple Criteria Decision Analysis (MCDA) or Multiple Criteria Decision Making (MCDM). A design algorithm, based on these ideas, is here proposed.

Example: Design and Control of a SISO Plant

Consider a SISO plant whose structure dictates that its transfer function should be of the form:

$$g(s) = \frac{a(s+b)}{(s+c)(s+d)} \tag{3.2}$$

where a, b, c and d are constants fixed through plant design.

Designing the plant on the basis of the steady state costs alone does not exclude the possibility of obtaining an unstable (c and/or $d<0$) plant with a RHP zero ($b<0$); A highly undesirable dynamic behaviour which the designer would try to avoid.

If an ideal conventional PID compensator is used to control the plant, then the controller transfer function is given by:

$$p(s) = (p_1 + p_2/s + p_3 s) \tag{3.3}$$

and the characteristic equation of the closed loop system is:

$$(1 + ap_3)s^3 + (c + d + ap_1 + abp_3)s^2 + (cd + ap_2 + abp_1)s + abp_2 = 0 \tag{3.4}$$

According to the Stodola criterion, MacFarlane [1970], for the system to be stable, the coefficients of the characteristic equation must be nonzero and of the same sign, say +ve:

$$1+ap_3>0 \tag{3.5}$$

$$c+d+ap_1+abp_3>0 \tag{3.6}$$

$$cd+ap_2+abp_1>0 \tag{3.7}$$

$$abp_2>0 \tag{3.8}$$

There are four inequalities and only three degrees of freedom (p_1,p_2,p_3). This means that depending on the plant parameters the above conditions may or may not be satisfied. In other words, for certain cases closed loop stability can not be achieved. This is indeed the case for the plant with a=1, b=-2, c=3 and d=-4. Inequalities (3.5) to (3.8) require $p_1>-1$ and $p_1<-6$ which is a contradiction.

This hypothetical example has served to illustrate two points.

(a) A final design obtained using the current approach to plant sizing might exhibit highly unfavorable dynamics.

(b) It is not always possible to improve the process dynamic behaviour through the use of a controller. In this case the plant could not be stabilised.

3.2.2 Dynamic Measures

Time delays, RHPT zeros, manipulated variables saturation and plant/model mismatch have been shown, in chapter 2, to be plant characteristics which limit the closed loop dynamic behaviour even if the best control system is used. Their effects, however, are dependent on the controllers used. In fact contrary to one's intuition the presence of these characteristics may lead to improved closed loop dynamic behaviour. In section 2.4, a SISO example is given where increasing the loop dead time and introducing a delibrate plant/model mismatch have resulted in an improved system behaviour. Holt and Morari [1985b] give a MIMO case where increased time delay has resulted in an improvement in the plant degree of controllabitly. In addition, the difficulty of developing sound generic quantitative measures of the process degree of controllability based on these attributes, particularly for the nonminimum phase elements (time delays and RHPT zeros), has been illustrated by the attempts of Holt and Morari [1985a&b], and Perkins and Wong [1985]. This suggests that until such generic measures are developed, if ever, the quality of control obtained from different plant designs will continue to be ranked using conventional, controller related indices.

Depending on the particular system considered, the dynamic criteria employed at the final plant design stage (plant sizing) may include open loop measures or closed loop measures, or a combination of both. An example is the design problem considered in chapter 6. A number of dynamic criteria, which include a measure of the open loop stability of the continuous stirred tank reactor (open loop damping) and a closed loop measure which is the Integral of Time multiplied by the Absolute Error (ITAE), are used.

3.2.3 MCDA and the proposed design algorithm

3.2.3.1 Multiple Criteria Decision Analysis (MCDA)

The theory of MCDA is concerned with the simultaneous maximization or minimization of a number of criteria subject to the problem equality and inequality constraints. Mathematically, this problem can be represented as:

$$\min_{x} \{F(x):D\} \tag{3.9}$$

where $F(x)=\{f_i(x)\}$ $(i=1,2,\ldots,k)$ is the vector of design criteria. These objectives are, usually, conflicting and noncommensurable. In the case of nonconflicting criteria this problem can be easily solved using any one of the traditional single objective function optimization techniques, since minimizing one criterion ensures that all the others are minimized. If the criteria are competing but commensurable then it may be possible to combine them into a single performance index using meaningful weights. The steady state design problem described in subsection 3.2.1 is an example of such a case. Due to the fact that both the operating costs and capital costs are measured in monetary terms (dollars or pounds), and that weights (cost factors) can be obtained through market analysis, the two criteria are combined to form a total cost function, $f_1(x)$. The best design, x_b, is chosen as the one which yields the lowest value of this function, i.e $(f_1(x_b)<f_1(x);\ x_b \neq x \in D)$. For the case where the different objectives are competing and noncommensurable, complete ordering of the feasible designs by the 'less than (<)' relation is not possible. However the set D can be partially ordered to yield a family of solutions to problem (3.9). This family of solutions is known as the pareto optimal, the noninferior, the efficient or the nondominated set. A solution $\hat{X}$ is noninferior if it is not possible to decrease any one of the objectives without simultaneously increasing the value of another, i.e there does not exist a feasible solution $\bar{X}$ such that:

$$f_i(\bar{X}) \leqslant f_i(\hat{X}) \qquad i=1,2,\ldots.,k$$

and $\qquad f_i(\bar{X}) < f_i(\hat{X}) \qquad$ for at least one i

During the last ten to fifteen years the literature on MCDA problems has grown at a high rate. A few techniques for generating the nondominated surface have been developed. These are, here, briefly reviewed. Also many attempts have been made into developing systematic methods which help the decision maker (designer) in choosing the best solution. These are dealt with in the books by Zenely [1982] and Goicoechea et al. [1982], and the review papers by Hwang et al. [1980], Clark et al. [1983] and Grauer et al. [1984].

3.2.3.2 Methods for generating the nondominated set

These techniques involve the conversion of problem (3.9) into a single criterion optimization problem, and most of them use the norm of the weighted vector of criteria F(x) as the objective function.

$$||WF(x)||_p = \{ \Sigma (w_i f_i(x))^p \}^{1/p} \qquad (3.10)$$

where w_i is a weighting factor of criterion $f_i(x)$, W=diag[w_i] (i=1,2,....,k), $w_i>0$ and $\Sigma w_i=1$. $1<p<\infty$ with p=1,2,∞ being the most useful norms.

<u>l_1 -norm (weighted sum) method</u>

Given a weighting matrix W, a nondominated solution is obtained by solving:

$$\min_x \{||WF(x)||_1 : D\} \qquad (3.11)$$

The entire set of noninferior solutions can be generated by systematically varying the weights, w_i's. The l_1-norm approach, however, has the drawback that, for a nonconvex problem, which is a characteristic of most chemical processes, some of the noninferior solutions can never be located, Hwang et al [1980].

<u>l_2 -norm technique</u>

Using p=2, the Eucledean vector norm, the difficulty with the l_1 -norm method in generating some of the noninferior solutions of nonconvex problems is removed.

$$\min_x \{||WF(x)||_2 : D\} \qquad (3.12)$$

The effective use of this approach requires that all the criteria must be nonnegative. This can be assured if the problem is reformulated as.

$$\min_{x} \{||WF(x)||_2 : D\} \qquad (3.13)$$

where,

$$F^{+}(x) = [f_i^{+}(x)] \quad i=1,2,\ldots,k ,$$

$$f_i^{+}(x) = f_i(x) - f_{i-}(x),$$

and

$$f_{i-}(x) \leqslant f_{i*}(x).$$

$f_{i*}(x)$ is the solution of:

$$\min \{f_i(x) : D\} \qquad (3.14)$$

A similar technique, described in detail by Grauer et al. [1984], is the "reference level" method:

$$\min \{-||F-\overline{F}||_2^2 + e||(F-\overline{F})_+||_2^2 : D\} \qquad (3.15)$$

where $\overline{F} = [\overline{f}_i]$, $(i=1,2,\ldots,k)$ denotes a reference vector of objectives (aspiration levels or goals). $(f_i-\overline{f}_i)_+ = \max\{0,(f_i-\overline{f}_i)\}$ and $e>1$ is a penalty coefficient. For convenience the argument x is dropped.

The solution of problem (3.15) is noninferior regardless of whether F is achievable or not. This formulation is much more useful than problem (3.12) in the sense that, more or less, only the desirable set of nondominated solutions can be generated as dictated by the aspiration levels.

l_∞ -norm technique

This problem is stated as follows:

$$\min_x \{\|WF(x)\|_\infty : D\} \tag{3.16}$$

which is equivalent to:

$$\min_x \{\max_i \{w_i f_i(x)\} : D\} \tag{3.17}$$

or

$$\min_x \{\gamma : D;\ w_i f_i(x) \leqslant \gamma \quad i=1,2,\ldots,k\} \tag{3.18}$$

or the goal attainment approach:

$$\min \{\gamma : D;\ w_i(f_i - \bar{f}_i) \leqslant \gamma \quad i=1,2,\ldots,k\} \tag{3.19}$$

Tabak et al [1980] applied this latter formulation, problem (3.19), to the design of an aircraft control system.

A common drawback of all the above techniques is the lack of a systematic approach for the variation of the weights w_i's or the aspiration levels. The work of Lightner [1979] highlights these difficulties.

Compromise programming technique

This technique is used for the generation of a portion of the nondominated surface or as a tool for helping the decision maker in choosing a particular solution. Compromise programming is based on the notion of distance from an ideal. Mathematically, this is defined as:

$$\min \{ ||F-F_*||_p : D\} \tag{3.20}$$

where $F_* = [f_{i*}]$ $(i=1,2,\ldots,k)$. f_{i*} is the solution of problem (3.14). F_* is known as the **ideal or utopian** solution.

For p=1, equal importance is given to all criteria deviations. In the space of the objective values, for p=2, the nondominated point from which the shortest line to the ideal point originates is considered to be the best solution. In the case of $p=\infty$, the maximum attribute deviation is minimized.

E- constraint method

This technique, which is useful for determining the complete nondominated surface of any system (convex or nonconvex), involves constraining (k-1) of the objectives and minimizing the kth criterion. By parametrically varying these (k-1) additional constraints the entire family of the noninferior solutions is obtained. The problem to be repeatedly solved for different sets of parameter values E_i's is:

$$\min \{f_1:D;\ f_i<E_i \quad i=2,\ldots,k\} \tag{3.21}$$

In the author's opinion, compared to the other approaches, this is a much better suited method for chemical and control engineering applications since it is simpler and allows the designer to have a direct say in the sought solution by choosing the levels of all the criteria but one. However, a systematic method for parameterically varying the bounds E_i's is lacking.

3.2.3.3 Proposed algorithm

A design algorithm, based on the E-constraint technique, which allows for systematic variations of the bounds E_is, is proposed. Also it ensures that only the most important portion of the noninferior surface is generated, and hence the effort required and problem complexity are reduced. This algorithm can be used not only for process design but for any problem whose solution calls for the simultaneous consideration of several criteria such as the determination of the best operating conditions of an existing plant/unit operation or controller design problems.

Step 1. Minimize the most important criterion. Usually this is the steady state cost function:

$$\min \{f_1:D\} \tag{3.22}$$

Note the levels of all the criteria at this problem solution x_*:

$$F^1 = (f_i^1) \quad i=1,2,\ldots,k \tag{3.23}$$

where,

$$f_i^1 = f_i(x_*)$$

Clearly if such a design exhibits a highly acceptable dynamic behaviour then x_* is the best solution and the design process is ended.

The criteria measuring the dynamic performance of the plant may or may not be known a priori. In any case, a detailed analysis of the minimum cost design will help the designer choose such objectives. It has to be mentioned that the plant control system, if not known a priori, is also fixed through such an analysis.

Step 2. Divide the vector of design criteria, F, into two sets. A primary set, $P=(f_1,f_2,\ldots,f_m)$ and a secondary set, $S=(f_{m+1},f_{m+2},\ldots,f_k)$. The former set is used to generate the nondominated surface, and hence the number of criteria it contains should be as small as possible. The secondary set is used to help the designer choose the best noninferior solution.

Step 3. If possible and desirable minimize a second primary objective, otherwise solve the following optimization problem:

$$\min \{f_1 : D;\ f_i \leqslant f_i^2;\ 1 \neq i \in m\} \qquad (3.24)$$

where $f_i^2 << f_i^1$.

Note the levels of all the criteria at the solution. If required readjust the P and S sets. The designer may decide to convert any objective into a conventional hard constraint which is then considered as a secondary criterion.

Step 4. Repeat step 2 for every primary criterion.

Step 5. Generate the nondominated set of solutions by repeatedly solving problem (3.25) below for different sets of bounds such that $f_i^2 < E_i < f_i^1$:

$$\min \{f_1 : D;\ f_i \leqslant E_i \quad i=2,3,\ldots m\} \qquad (3.25)$$

The choice of E_i's may be systemised by repeatedly solving the following problem instead of problem (3.25)

$$\min \{f_1 : D;\ f_i \leqslant f_i^2 + n_i E_i \quad i=2,3,\ldots m\} \qquad (3.26)$$

for the different vectors $N=[n_i]$ $(i=1,2,\ldots,m)$. Where n_i assume any of the integer numbers between

0 and r_i inclusive. r_i is a small integer number chosen by the designer. It should be large enough to allow the prediction of the entire noninferior surface from the generated solutions. E_i is given by:

$$E_i = (f_i^1 - f_i^2)/r_i \quad i=1,2,...m \tag{3.27}$$

This systematic approach is particularly useful when the number of primary criteria is greater than two.

Step 6. By analysing the noninferior surface and the tradeoffs required, the designer may be able to reject most of the possible solutions. Evaluation of the secondary criteria for the set of promising designs allows him to choose the best solution.

CHAPTER 4

OPTIMIZATION METHODS AND SIMULATION PACKAGES

In this chapter, a number of tools used in this study are briefly described. These are the direct-search optimization techniques of Box [1965], and Hooke and Jeeves [1961], and the continuous system simulation packages ISIM and TUTSIM. The optimization methods are considered in section 4.1 and the simulation packages are treated in section 4.2.

4.1 Optimization methods

The form of a general nonlinear optimization problem is given by equation (3.1) which can be rewritten as:

$$\min_{x}\{f(x):h(x)=0,g(x)\geqslant 0\} \tag{4.1}$$

or

$$\min_{x}\{f(x):h(x)=0,x_L\leqslant x\leqslant x^U,g_i(x)\geqslant 0 \quad \text{for} \quad i=2N+1,2N+2,\dots\dots,p\} \tag{4.2}$$

where x is the vector of N decision variables, f(x) is the objective function to be optimized and h(x)=0 is the set of equality constraints. g(x) is a p-dimensional vector of functions defining 2N explicit and (p-2N) implicit inequality constraints. x_L and x^U are, respectively, vectors of lower and upper bounds on the decision variables.

Note that a maximization problem can easily be converted to a minimization problem since $\max\{f(x)\}=\min\{-f(x)\}$.

A large number of techniques are available for solving the above general optimization problem or the special cases evolving from it. Two such methods, which have been used in this investigation, are described in the following two subsections. These are the "complex" technique of Box [1965] and the pattern search technique of Hooke and Jeeves [1961]. These two direct search methods have enjoyed wide application in a number of engineering fields.

4.1.1 The complex method

The complex (constrained simplex) method was developed by Box [1965] from the simplex method of spendley et al. [1962]. It was devised for solving nonlinear constrained optimimzation problems of the form given by equations (4.1) or (4.2). Inequality (explicit and implicit) constraints are handled by the use of a flexible figure which has k vertices. Where $k \geq N+1$. This figure, which is referred as the "complex", can be expanded or contracted in any or all directions and can be extended around corners.

The initial complex consists of a given feasible point, and (k-1) points generated from random numbers and the upper and lower bounds on the decision variables as:

$$x = x_L + r(x^U - x_L) \tag{4.3}$$

where r is a vector of random numbers in the interval (0,1).

If a generated point violates an implicit constraint, it is moved half-way toward the centroid of the other already selected feasible points. This process is repeated until all the vertices of the complex are defined. The centroid , x_c, of m points is calculated as:

$$x_{i,c} = (1/m)\sum_{i=1}^{m} x_{i,j} \tag{4.4}$$

where i refers to the coordinate and j refers to the point.

The objective function is then evaluated at each vertex of the complex. The point yielding the poorest functional value is rejected and replaced by a new point given by:

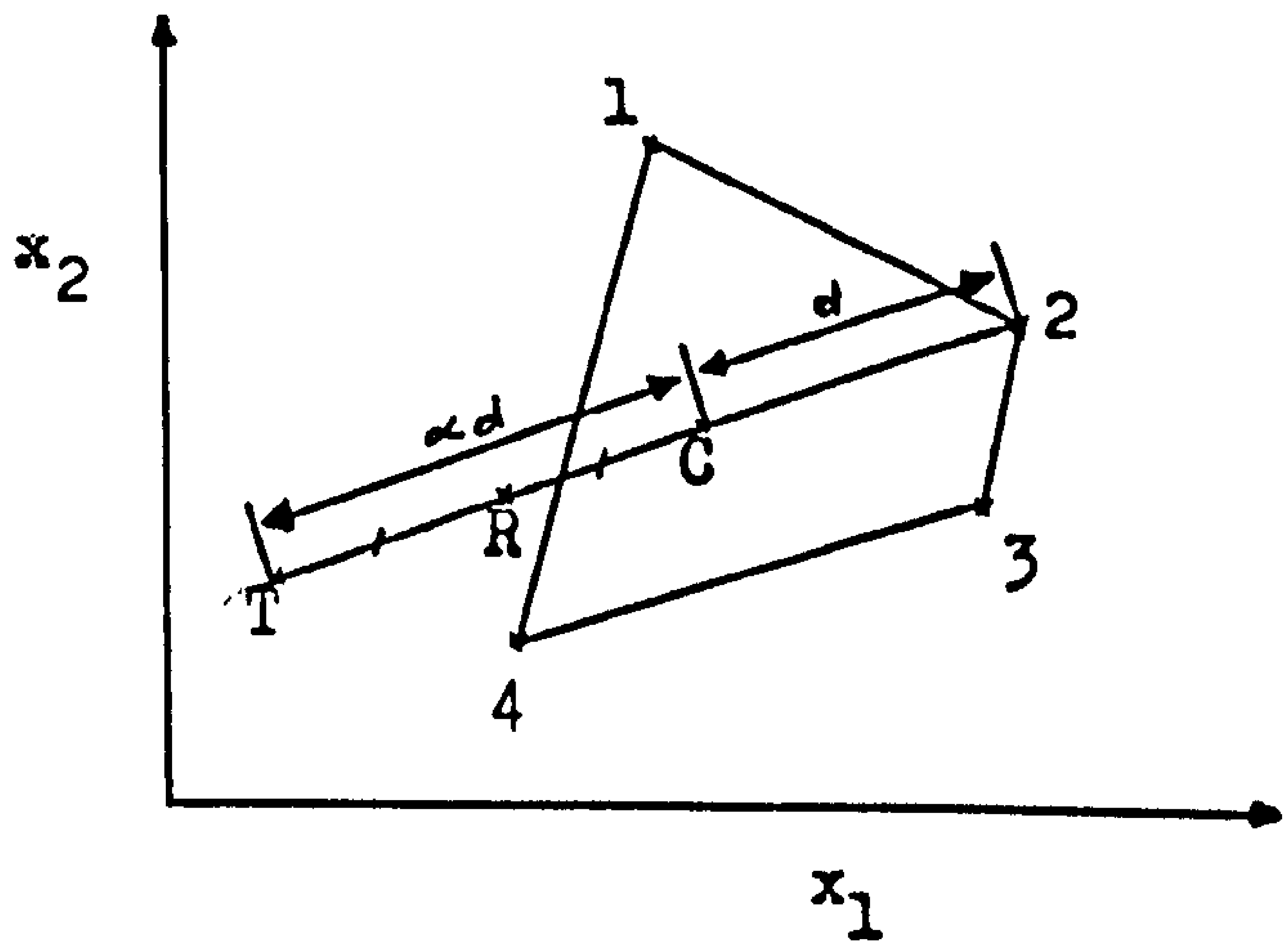
$$x_{new} = \alpha(x_c - x_{old}) + x_c \tag{4.5}$$

where x_{new} and x_{old} are the new and rejected points respectively. α is a positive number greater than 1.

At the new point, the objective function and the constraints are calculated. Depending on the outcome of these calculations a number of possible actions may be taken:

(a) The new point is feasible and its corresponding objective function value is not the poorest of the set of k points. In this case, identify the worst point and continue with a reflection using equation (4.5).

(b) The new point is feasible and its functional value is the worst of the current set of k points in the complex. Retract this point by half the distance to the previously calculated centroid (see figure 4.1). The retraction



: $k=4$, $\alpha >1$.

: Point 2 is the worst point

: Point C is the centroid of points 1, 3 and 4

: Point T is the result of reflecting point 2

: Point R is the result of retracting point T

Figure 4.1 A hypothetical two-dimensional example illustrating the main features of the complex optimization method.

procedure is continued until a point which is better than at least one of the other (k-1) points is obtained.

(c) The new point violates one or more of the bounds on the decision variables. Reset the coordinates in question at their limits (or a certain distance inside their limits) to yield a feasible point. Continue as in (a) or (b) depending on the value of the objective function corresponding to this new feasible point.

(d) The new point does not satisfy one or more implicit constraints. retract this point by half the distance to the centroid of the remaining (k-1) points. The retraction technique is continued until a feasible point is obtained.

Progress will continue with repeated rejections and regenerations until the complex is reduced essentially to the centroid. The search is terminated when five consecutive function evaluations give equal values of the objective function to within a certain accuracy.

During the search the complex rolls over and over, normally expanding, until the optimum solution is bracketed or a boundary is reached. When the latter case occurs, the complex contracts and flattens itself against this constraint. It can then roll along the boundary and leaves it if the contour is changed.

Values of α, the reflection factor, greater than one cause a continued expansion of the complex and compensates for moves half-way toward the centroid. The expansion of the complex increases the probability of obtaining a global minimum value of the objective function. Box [1965] performed a limited number of numerical experiments with this algorithm, and on this emperical basis recommends using $\alpha=1.3$ and $k=2N$.

There are two distinctive situations in which the complex optimization algorithm fails.

(a) For a nonconvex problem, there is no garantee that the centroid of a set of feasible points is feasible.

(b) If the corrected point, the centroid of the remaining (k-1) complex points, and every point on the segment joining these two points all have functional values lower than the functional values at each of the remaining (k-1) points of the complex, the algorithm will result in an infinite loop.

In this study, this optimization algorithm has been modified such that if any of these two situations arises, the best vertex of the complex is used as a temporary centroid of the vertices of the complex other than that point yielding the worst value of the objective function.

The complex algorithm assumes that a starting feasible point is available. However,such a point can also be generated in a similar way as the remaining (k-1) points in the initial complex. A trial point is generated using a pseudo-random number generation routine and equation (4.3). This point can then be tested for feasibility by evaluating the implicit inequality constraints. Such a process is repeated until a feasible point is obtained. This is a useful approach if a large number of different feasible points is sought. In some cases, however, this automatic approach to the generation of a starting point can require an extensive computation time.

A computer program which implements the modified complex method of Box [1965], is given in the software appendix at the end of this thesis. This program, which consists of a number of subroutines, is based on Algorithm 454 of the Association of Computing Machinery (ACM), [Algorithm 454, collected algorithms from the ACM, 1980].

4.1.2 The Hooke and Jeeves (HJ) pattern search method

The Hooke and Jeeves [1961] optimization method is an unconstrained direct search technique. It is based on two simple strategies, referred to as "exploratory" and "pattern" moves. The exploratory moves are aimed at examining the local behaviour of the function being optimized and gathering information concerning the best direction for improvement. The pattern move uses this information to step rapidly along the valleys, if any, and hence accelerates the speed of convergence.

An exploratory move is completed by introducing a step change in the value of a single decision variable and checking whether such a change is a success or a failure. A move is termed a success if the value of the objective function decreases. The new point is retained only if it is a success, otherwise the step is retracted and replaced by a step in the opposite direction which, in turn, is retained depending upon whether it succeeds or fails. An exploratory search is completed after all the decision variables have been investigated. Such a search is considered successful if it yields a point better than the base point. A base point is here defined as the starting point or the point from which the pattern move has been made. A successful exploratory search is followed by a pattern move to yield:

$$x_p = x_b + (x_b - x_{b-1}) \tag{4.6}$$

where x_b, x_{b-1} and x_p are, respectively, the current base point, the previous base point and the pattern move point.

x_p then becomes the point from which an exploratory search is conducted. If this search is successful the best point, obtained thus far, is accepted as the new base point and another pattern move is performed followed by an exploratory search. This sequence is continued until the exploratory search fails. In this case, another exploratory search is undertaken from the current base point x_b. If this second search fails the step sizes are reduced by some factor and the exploration is resumed. The search is terminated when the step sizes fall below some prespecified magnitudes.

An example illustrating the operation of this optimization method is presented in figure 4.2. The numbers

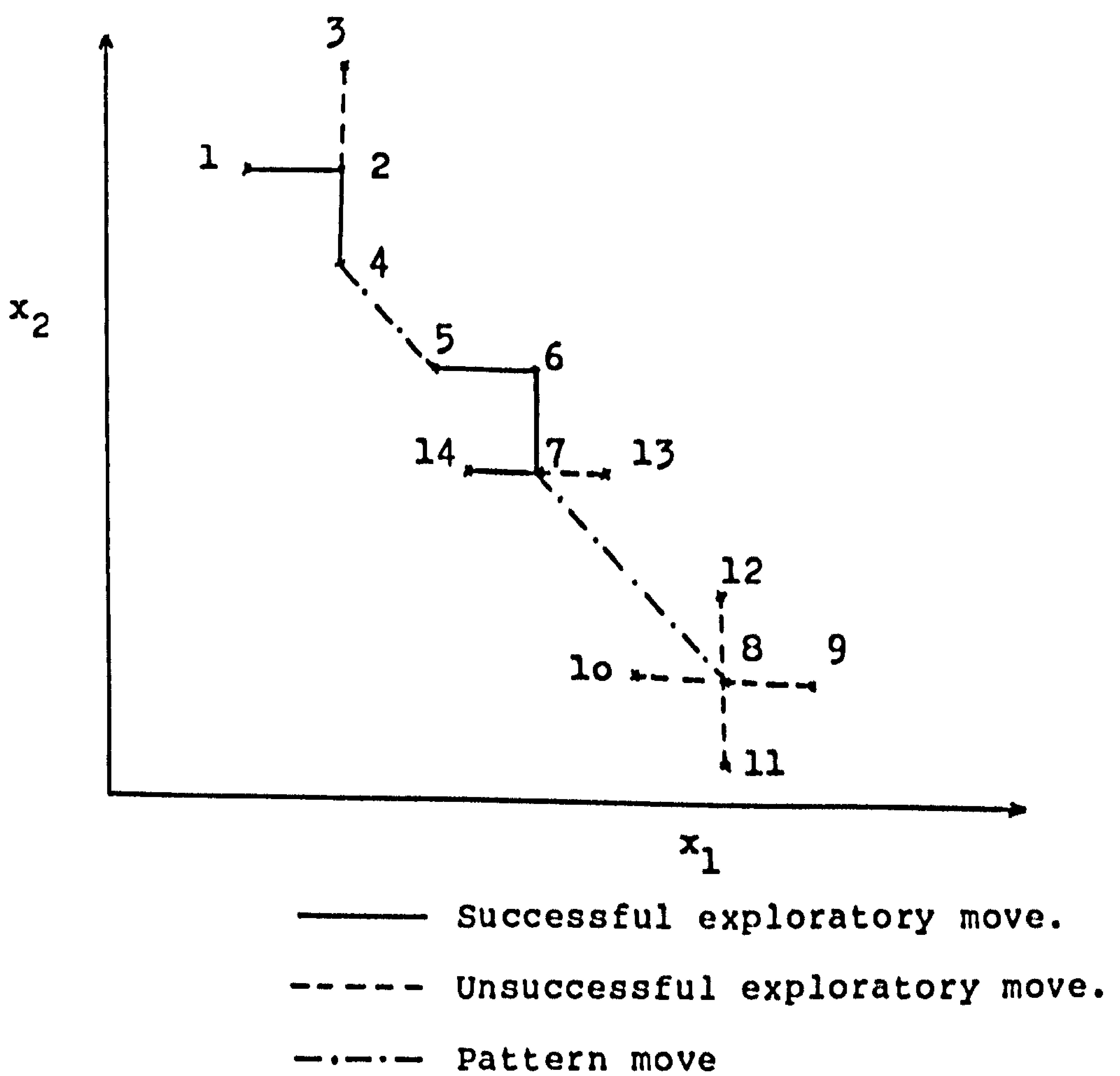


Figure 4.2. A hypothetical example illustrating the Hooke and Jeeves method

indicate the sequence in which the points are selected. Points 1 (the starting point), 4 and 7 are base points. Notice that it is assumed that the algorithm remembers the last successful exploratory coordinate directions.

A detailed flowchart of the algorithm can be found in the original paper of Hooke and Jeeves [1961]. Algorithm 178 of the ACM, [Collected Algorithms from the ACM, Algorithm 178, 1980], is an ALGOL computer program which implements a slightly modified version of this flowchart. An ISIM version of this program, which is used in chapters five and six, is given in the software appendix at the end of this thesis.

As stated earlier, the direct search method of HJ has been devised to solve unconstrained optimization problems. But the controller design problems considered in this study may involve the minimization of an objective function subject to a number of explicit and implicit constraints on the decision variables (controller parameters). Such constraints, however, can be easily accommodated through the use of barrier or penalty functions which involve the conversion of the constrained optimization problem given by equation (4.1) to the following unconstrained minimization problem:

$$\min\{f(x)+ \psi[e,g(x)] \ : \ h(x)=0\} \qquad (4.7)$$

where e is termed the vector of penalty parameters and ψ, the penalty term, is a function of e and g(x).

ψ is chosen such that feasible points are highly favored over imfeasible points. A number of penalty functions are commonly used. The interested reader is referred to chapter 6 of the book on "Engineering Optimization Methods and Applications" by Reklaitis et al. [1983]. In this study, the penalty function referred to as the bracket operator has been employed. It is defined as:

$$\psi = \sum_{i=1}^{p} e_i \langle g_i \rangle^2 \tag{4.8}$$

where,

$$\langle n \rangle = \begin{cases} n & \text{if} \quad n \leqslant 0 \\ 0 & \text{if} \quad n > 0 \end{cases} \tag{4.9}$$

Equation (4.8) may be used to accommodate implicit and explicit (simple bounds on the decision variables) constraints. A second method which can be employed for correcting for explicit constraints violation is the simple technique recomended by Box[1965]. This technique calls for resetting the decision variables, which do not satisfy the constraints, at their limits to yield a feasible point. A number of optimization problems have been successfully solved using the HJ method with the latter technique employed as a correction measure for simple bounds violation.

4.2 Simulation packages

4.2.1 TUTSIM for the Apple II microcomputers

TUTSIM is a block-oriented continuous system simulation package. The Apple II version of TUTSIM is written in assembler language for a 6502 processor on which the Apple II microcomputers are based. Some of the features of this package are:

(a) Incorporated in the package is a simple editor which allows code to be input directly from the keyboard with instant syntax checking and error reporting on a line-by-line basis.

(b) The system model is entered into the microcomputer and run interactively using a simple set of commands.

(c) A simulation run can be interrupted during execution so as to pass control to the user. At this stage, the programmer may wish to check the values of some variables and make certain changes. Execution can then be restarted or, in certain cases, continued from the point of interruption.

(d) The system model can be saved on a floppy disc for later use.

(e) The results can be obtained in either numerical or graphical format.

(f) The system model is programmed in the same way as it is solved on an analog computer, i.e block diagram form, using a library of standard function blocks. The library is constructed of over 30 algebraic linear and nonlinear block functions which include two integration methods: Euler and the Adams-Bashforth algorithm, a practical PID controller, limiters and a first order lag block.

(g) The package uses floating-point arithmetic. This means that the need for variable scaling is eliminated.

(h) Since the package is written in assembler language, it is fast.

The shorcomings of TUTSIM include:

(a) Comments can not be included in the code representing the system model.

(b) The results of a simulation run can not be saved.

(c) Graphs are not labeled which could be confusing when a number of similar signals are plotted simultaneously.

Example: Simulation of a simple control loop

The simulation of a system which consists of a first order plant and a proportional feedback controller is here considered. The transfer function of the plant is given by:

$$\frac{Y(s)}{U(s)} = \frac{2}{3s + 1} \tag{4.10}$$

and the controller gain, p_1, has a value of 1.5. The system input is assumed to be a unit step change in the set point.

Using these information, the TUTSIM block diagram representation of the system, the code listing and the simulation results are as shown Figure 4.3.

A full description of the TUTSIM language and its features can be found in the TUTSIM user manual*.

4.2.2 ISIM

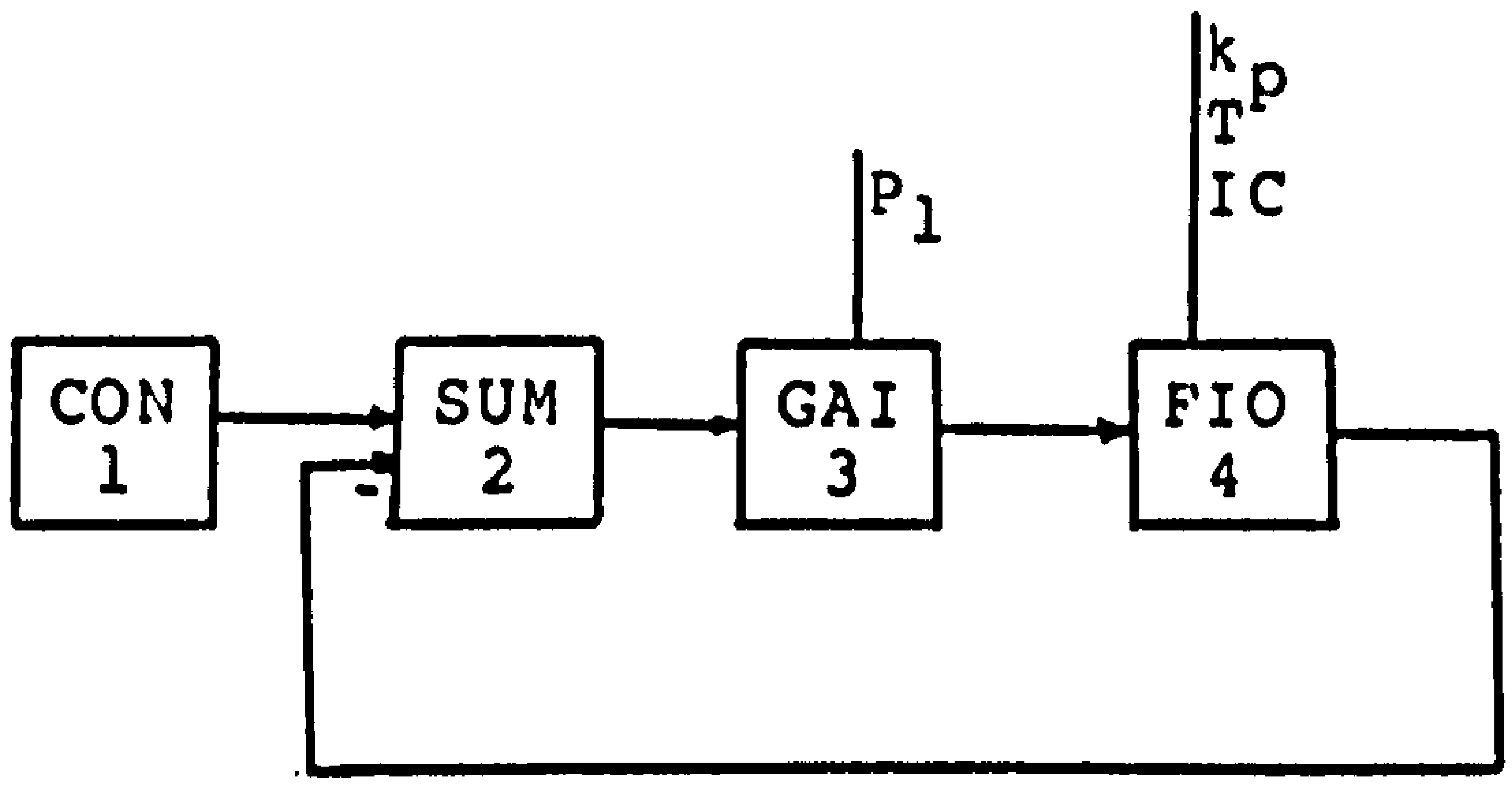
ISIM is an interactive simulation package for use in the building of computer models of continuous dynamic systems. It runs on CP/M, MS or PC-DOS systems such as the Apple II and IBM PC microcomputers. ISIM has been adapted from the earlier language, ISIS which was developed for minicomputers. Like most Continuous System Simulation Languages (CSSL's), it is an equation-oriented package.

The structure of CSSL recommended by the Simulation Councils+, upon which the ISIM package is based, is as shown in figure 4.4. The program is divided into three regions known as the INITIAL, DYNAMIC and TERMINAL regions. The INITIAL region contains the equations required prior to execution of the model, the DYNAMIC region contains the

* "TUTSIM user manual", Process Automation and Computer Systems Ltd., Graphics House, 50 Gosport Street, Lymington, Hants SO4 9BE.

+ The Simulation Councils Continuous System Simulation Language, Simulation, Vol. 9, No. 6, December 1967.

TUTSIM BLOCK DIAGRAM



TUTSIM CODE LISTING

```
TIMING
 0.40000E-02   0.30000E+01

OUTPUTBLOCKS AND RANGES
X1:      0       0.00000E+00   0.30000E+01
Y1:      1       0.00000E+00   0.15000E+01
Y2:      3       0.00000E+00   0.20000E+01
Y3:      4       0.00000E+00   0.15000E+01

MODEL
 0.10000E+01        1 CON
                    2 SUM       1     -4
 0.15000E+01        3 GAI       2
 0.20000E+01        4 FIO       3
 0.30000E+01
 0.00000E+00
```

TUTSIM RESULTS

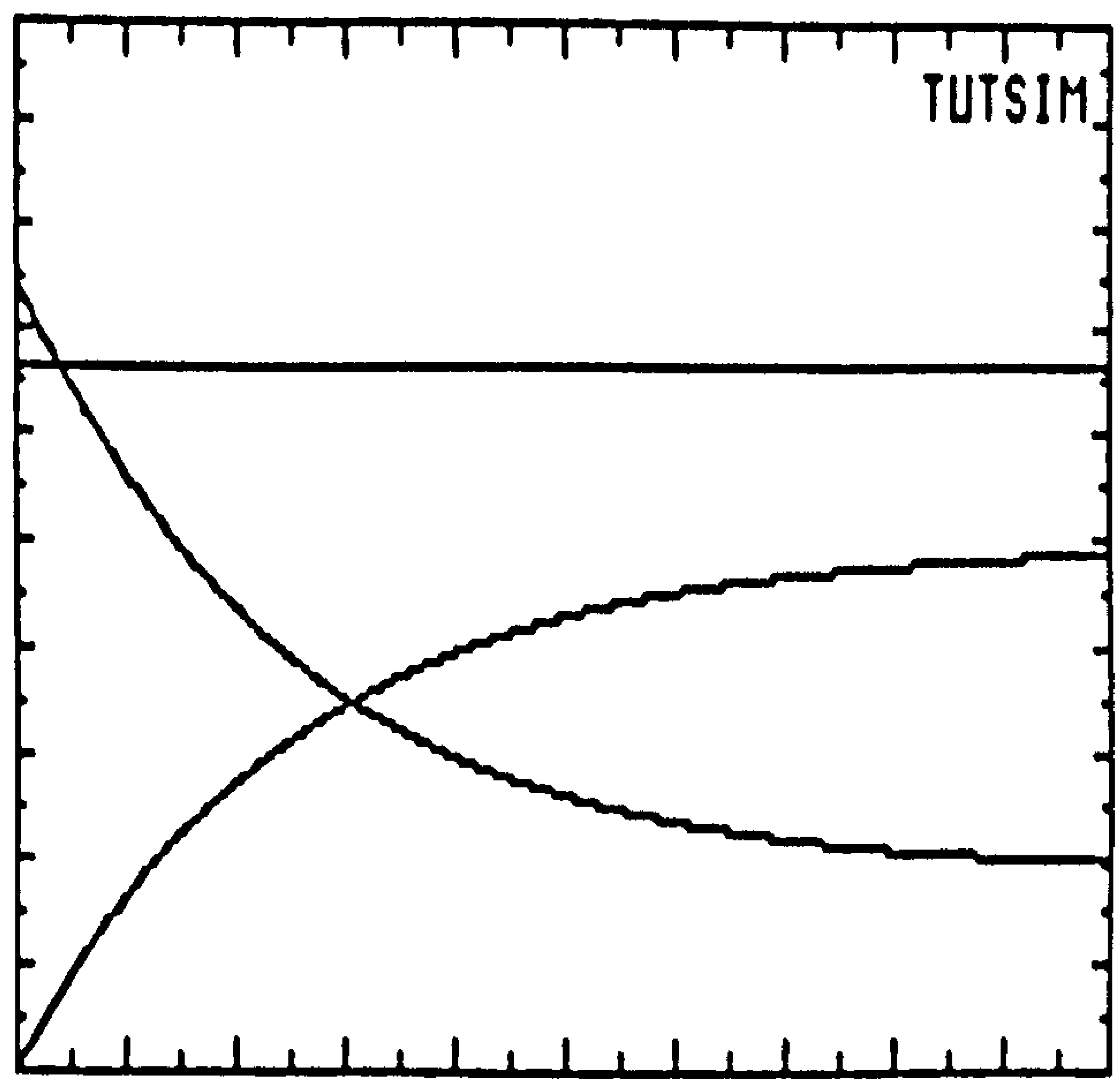
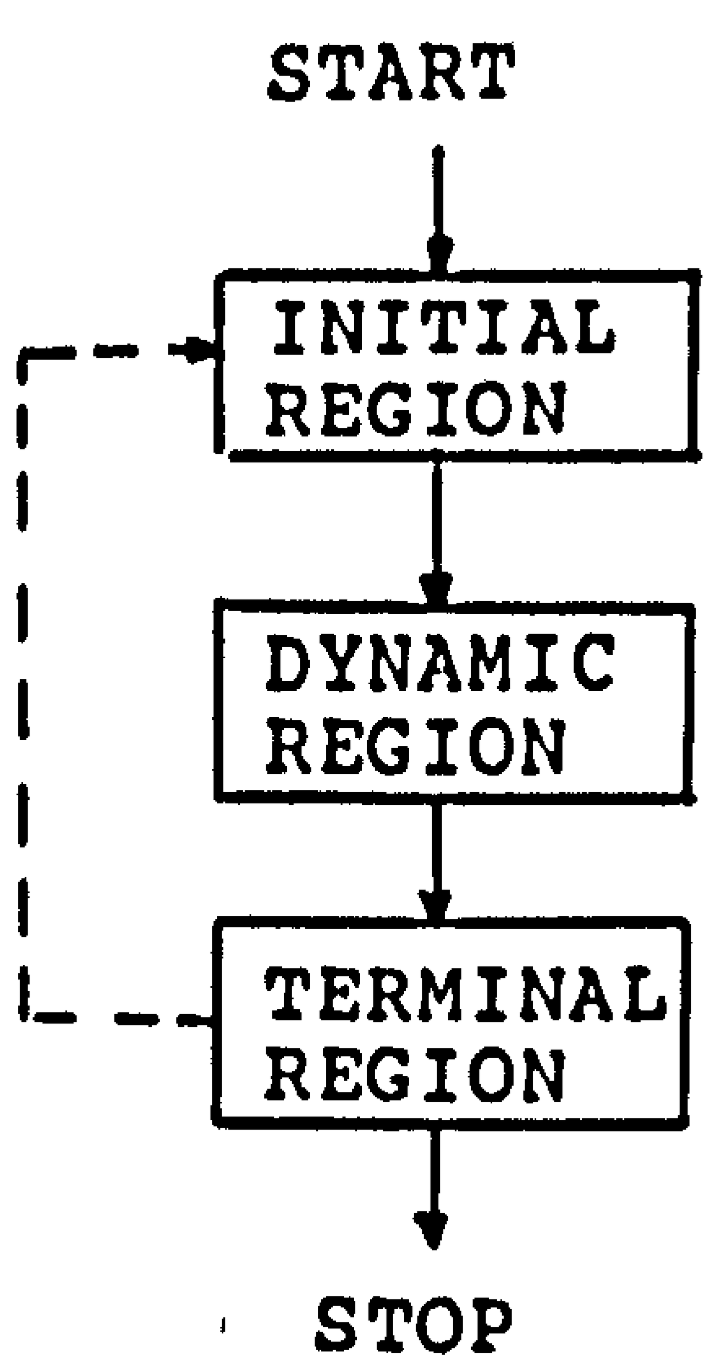


Figure 4.3 Simulation of a simple feedback loop using TUTSIM

differential and other algebraic equations describing the model and the TERMINAL region contains any equations required to do post-processing on the solution. In normal use, a simulation run would involve a single pass through the INITIAL region, then the DYNAMIC region is repeatedly executed until the solution is complete and a single pass through the TERMINAL region. The program is then terminated or a return to the INITIAL region is made for further runs.

In ISIM/ISIS/ISIS80 this CSSL structure has been extended by a fourth region known as the CONTROL region, figure 4.5. This region is similar to the main root in a FORTRAN program. Its purpose is to define the experiments to be carried on the system model. The latter may be called from the CONTROL region by a SIM statement. On completion of the simulation run, control is returned to the statement



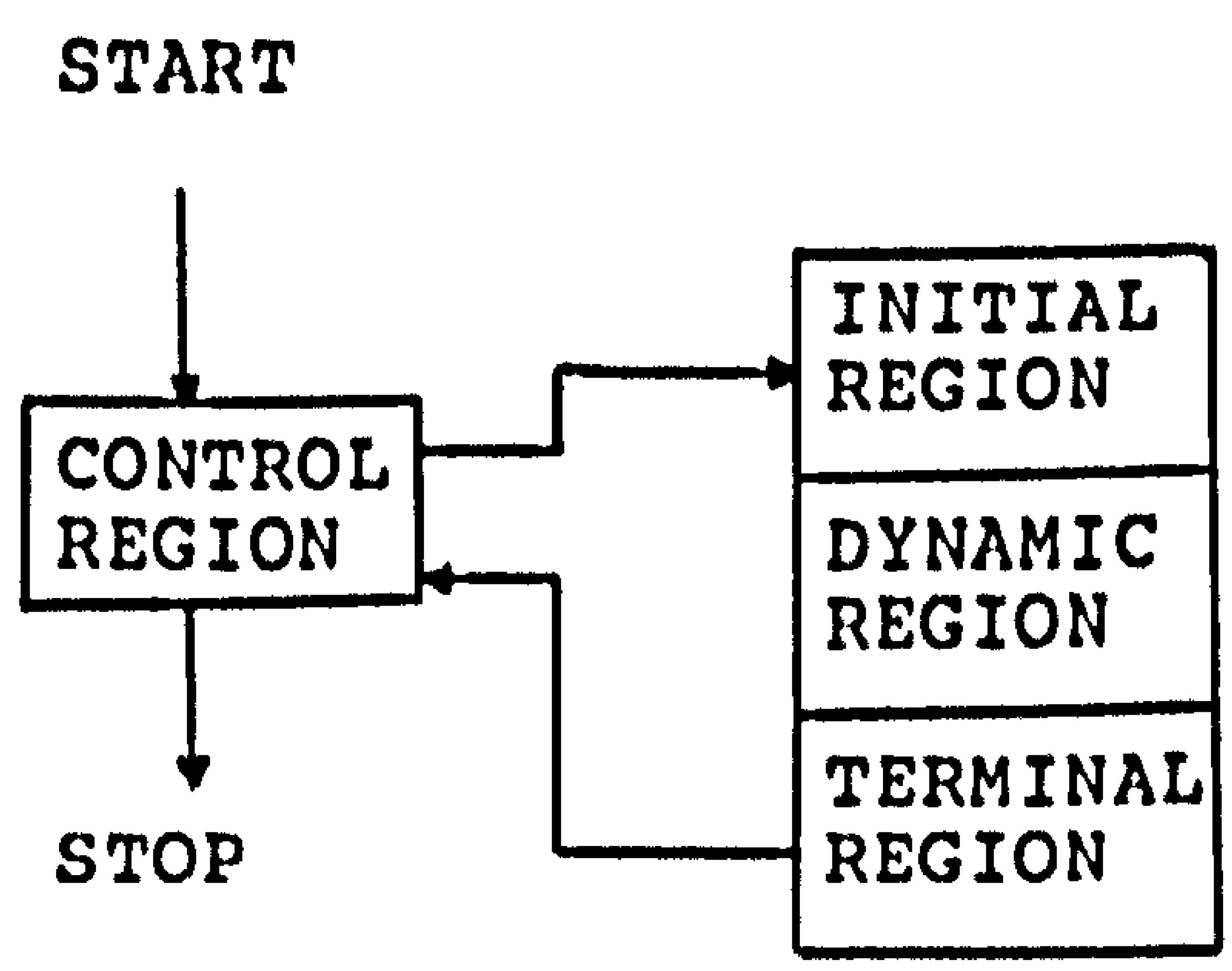


Figure 4.4 Standard CSSL structure.

Figure 4.5 ISIS/ISIS80/ISIM structure.

following the SIM statement. The implementation of an optimization algorithm such as the HJ method is made possible by the the addition of the CONTROL region in the ISIM structure.

Features (a) to (f) of the TUTSIM package listed above are also features of the ISIM package. Other characteristics of the ISIM package include:

(a) The results of a simulation run can be saved on floppy discs.

(b) The package provides a choice of three integration methods, namely the second order and fourth order Runge Kutta, and a fifth order variable step Runge Kutta.

(c) A line of code may contain more than one statement.

The drawbacks of ISIM include:

(a) Since it is an interpreted language written in FORTRAN, ISIM is relatively slow.

(b) Although arrays can be used in ISIM, a number of operations can not be performed on their elements.

(c) An arithmetic overflow returns control to the operating system monitor rather than the ISIM monitor, which makes it difficult to debug the program in question.

The negative feedback control loop simulated in subsection 4.2.1 using the TUTSIM language is also simulated in this subsection using the ISIM language. In the time-domain the considered plant, equation (4.10), has the following representation:

$$3 \frac{dy(t)}{dt} + y(t) = 2u(t) \tag{4.11}$$

$$y(0) = 0 \tag{4.12}$$

The ISIM code listing and the simulation results are as shown in figure 4.6. Again, the reader is referred to the ISIM user manual* for a detailed description of the ISIM language.

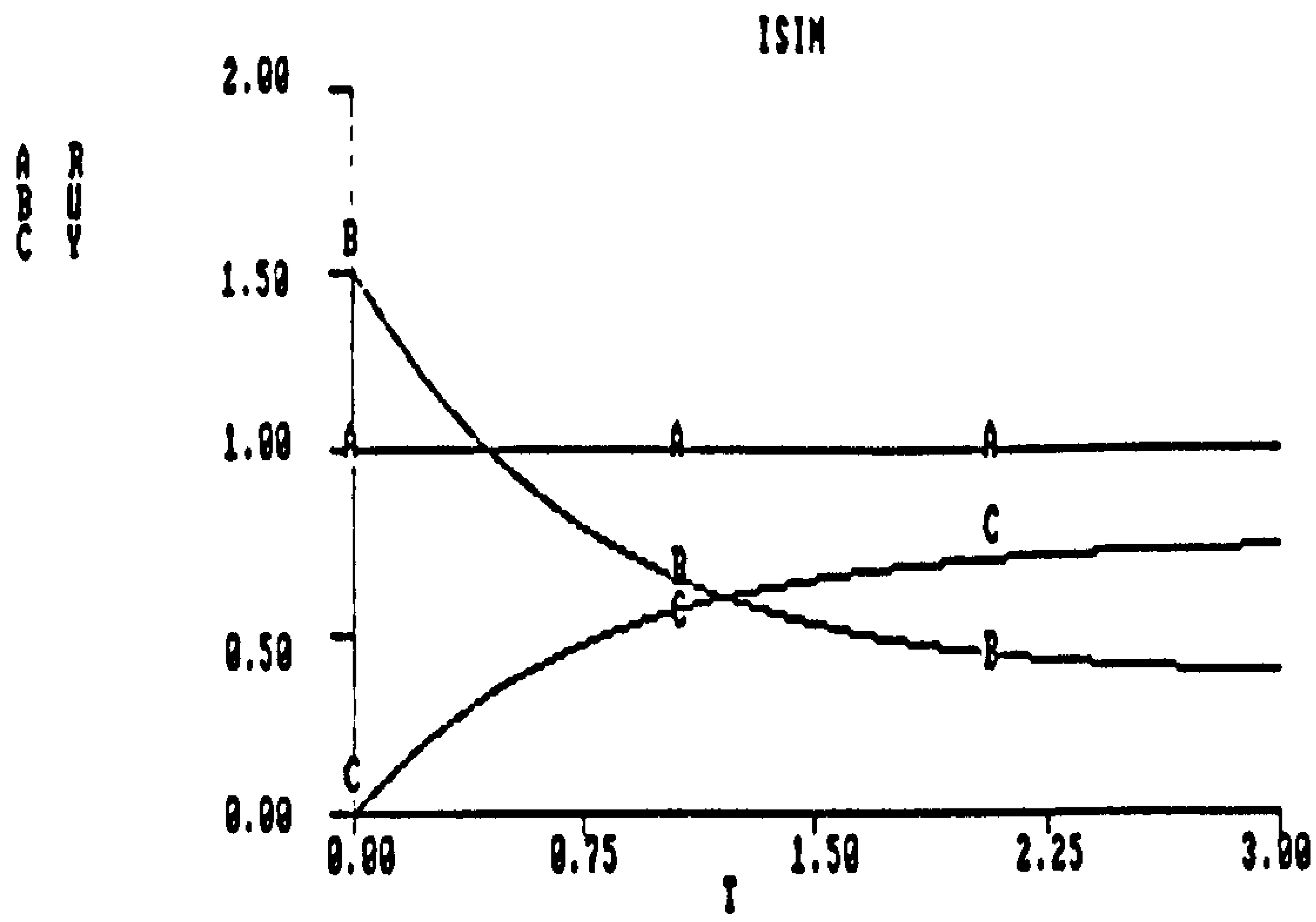
---

* "ISIM Interactive Simulation Language User Manual". Available from Simulation Systems, The Gables, North End, Yatton, Bristol, BS19 4AF, UK.

ISIM CODE LISTING

```
: ==== Simulation of a simple control loop ====
:
: control region
:
    tfin=3; cint=0.004
    r=1; sim
:
: model description
:
 initial
      y=0; y'=0
dynamic
     e = r-y                          : controller input (error)
    u = 1.5*e                         : controller output
     y'= (2*u - y)/3                  : plant model
     prepare t,r,u,y
     output t,r,u,y
# VAL ALGO    =   1.0000
```

ISIM RESULTS



Remain in Graphic Mode (Y/N) :

Figure 4.6 Simulation of a simple control loop using ISIM

CHAPTER 5

DESIGN of SISO FEEDBACK CONTROLLERS - A MULTIOBJECTIVE APPROACH

5.1 Introduction

Single loop Proportional plus Integral plus Derivative (PID) controllers and their variants are widely used in industry. This popularity is due not only to their simplicity and reliability but also to their high effectiveness. This latter quality is stressed by the fact that a number of controller design techniques have been found to lead to conventional PID controllers. In optimal control theory the solution of the Linear Quadratic Problem (LQP) is a proportional state feedback controller. Integral action can also be obtained through solving a modified LQP formulation, O'Connor and Denn [1972]. Recently, Morari et al. [1984] have found that, in many cases, The Internal Model Control (IMC) design procedure, which is based on the notion of perfect control, also leads to conventional PID controllers.

During the years many approaches for the design of single loop controllers have been developed. Examples include Lopez et al [1967], Cohen and Coon [1953], and Ziegler and Nichols [1942] methods. Due to the fact that most of these techniques are based on an overall performance index, the characteristics of the closed loop dynamic behaviour obtained vary from case to case.

Realising this and other drawbacks, Zakian and Al-Naib [1973], and Zakian [1979] reformulated the controller design problem as the solution of a set of inequalities. These inequalities are functionals describing the closed loop system behaviour. To find a solution which satisfies the set of hard constraints, they proposed a technique known as the Moving Boundary (MB) method. Two shortcomings of this approach are that the solution obtained is highly dependent on the starting point and that the designer is asked a priori to state the desired levels of the different functionals (criteria). If during the solution process it becomes clear to the designer that his goals are unachievable then he can reformulate the problem by defining new aspiration levels. This process is continued until a satisfactory solution is obtained. The designer, however, is much more likely to make the right decision concerning the choice of the best design if he is given, a priori, some or all of the information on what is achievable and the tradeoffs involved, e.g the required percentage increase in the rise time for a one percent decrease in the overshoot. This means the generation of the nondominated surface. As indicated in section 3.2 the proposed design algorithm is suitable for such an activity. This algorithm is here applied to the design of SISO controllers.

Twenty years ago the designer might have been put off when considering the time and effort required for the use of such a technique. Today, the widespread availability of high speed computers and interactive continuous system simulation packages have altered the picture completely. A few minutes may be enough to perform the entire design activity. If the system considered is linear, then the use of the numerical inversion of the transfer function technique of Zakian [1969] instead of the well known integration methods, which are comparatively speaking quite slow, will spead up the simulation process considerably.

The remainder of this chapter is organised as follows. In section 5.2, some of the available methods for the design of conventional PID controllers are briefly reviewed. For design purposes, the criteria by which the closed loop system response is normally judged are given in section 5.3. The application of the proposed multiobjective design approach is considered in section 5.4, and a brief discussion of the obtained results is given in section 5.5.

5.2 Available Design Methods

The available techniques for the design or tuning of SISO PID family of controllers are divided into three main categories, namely frequency domain, s-domain and time domain methods.

5.2.1 Time domain methods

The time domain methods are classified either as open loop or closed loop techniques. Most of the open loop methods rely on the presence of a simple plant model, usually a First Order PLus Dead Time (FOPDT) model.

5.2.1.1 Open loop techniques

Based on an overall performance index, many workers have developed correlations which relate the optimal controller parameters to the plant model parameters. These correlations are given either in graphical or equation forms. The commonly used performance indices are the quarter decay ratio, the Integral of the Squared Error (ISE), the Integral of the Absolute Error (IAE) and the Integral of Time multiplied by the Absolute Error (ITAE). References to several of these tuning relations are given in Appendix 5A. These approaches have many drawbacks which include:

(a) For the majority of the control loops in the chemical and petrochemical industries a quarter decay ratio response is considered to be too oscillatory.

(b) Most of the open loop techniques are based on an approximate FOPDT plant model. The performance of the real plant, which is usually of high order, differs considerably from that of its approximate FOPDT model for which the optimal controller is designed. The work of Weigand and Kegerreis [1972] clearly illustrates this point. These workers have found that the methods derived on the basis of a FOPDT models to be too conservative when applied to Second Order Plus Dead Time (SOPDT) plants.

(c) The settling time, rise time and overshoot are the closed loop characteristics by which the time responses are judged. If any of the methods in this class is used for controller design then the obtained values of these attributes and the tradeoffs involved will be found to differ from case to case as shown in table 5.1 where PI controllers are designed for FOPDT plants with different time delay to time constant ratios. The controllers are tuned using Rovira et al. [1969] IAE relationships. Depending on the particular application, the optimum closed loop dynamic behaviour of a plant with a ratio of time delay to time constant equal to one might be considered too sluggish whereas that of a plant with a ratio of time delay to time constant equal to 0.1 might be considered to exhibit a high overshoot and to require a large control effort.

(d) Some techniques are based on load disturbance inputs which enter the loop at a particular location. The loop performance might be highly impaired if for the plant in question the major loads enter at a different location.

attribute* / R	t_1	t_2	m_p	$\|u\|_{max}$
0.1	0.29	0.62	0.076	6.04
0.3	0.76	2.20	0.128	2.69
0.5	1.20	3.80	0.125	1.92
0.8	1.90	5.80	0.076	1.44
1.0	2.48	6.80	0.029	1.26

Table 5.1: Characteristics of the optimal+ closed dynamic behaviour of the plant:

$$g(s) = \frac{e^{-T_d s}}{Ts+1} \quad \text{with } T=1$$

and $R=T_d/T$

\+ The controller is a PI tuned using Rovira et al. [1969] minimum IAE relationships.

* These attributes are defined in section 5.3

5.2.1.2 Closed loop techniques

A large number of methods belong to this category of controller design techniques. Examples are the direct optimization method in which a scalar performance index such as the ISE is minimized, subject to the closed loop behaviour equality and inequality constraints, to yield the optimal controller parameters; the method of inequalities which is briefly described in section 5.1; and the popular Continuous Cycling (CC) method proposed by Ziegler and Nichols [1942]. Due to its widespread popularity and the fact that it has been used in this investigation, a brief account of this latter technique is given in the remainder of this subsection.

The CC method involves the determination of the largest gain of a proportional controller for which the closed loop system is stable. In other words, the determination of the gain which causes the loop to continuously oscillate and hence the naming continuous cycling method. This gain is referred to as the ultimate gain and the period of the system response associated with it is termed as the ultimate period. Ziegler and Nichols proposed relationships between the optimal parameters of the PID conventional controllers and these two characteristics. They used the quarter decay ratio criterion as the performance index. These relationships are given in Appendix 5A. The CC method has the disadvantage that a too oscillatory response is obtained. In addition, for certain cases, it yields an unstable system.

5.2.2 Frequency domain methods

Frequency response methods employ the sinusoidal response of the open loop (controller plus plant) and closed loop systems to predict reasonable values of the controller parameters.

The open loop frequency response methods are based on the Bode and Nyquist stability criteria. Bode criterion states that a control system is unstable if the open loop frequency response exhibits an amplitide ratio (output-input ratio) exceeding unity at the critical frequency (frequency corresponding to 180^{o} phase lag). This criterion applies only to systems for which the Bode plots decrease monotonically with frequency. The Bode plots are a pair of diagrams showing the logarithm of the amplitude ratio and the phase shift versus the frequency. Another stability criterion which does not place any restrictions on the shape of these curves is that of Nyquist. The latter is based on the polar plot of the output-input ratio with the frequency as a parameter. This plot is also referred as the Nyquist plot. The Nyquist stability criterion states that the number of RHP zeros of the characteristic equation (poles of the closed loop system) of a given system is equal to the number of clockwise encirclement of the (-1,0) point by the Nyquist plot of the open loop transfer function as the frequency varies from $-\infty$ to ∞.

In both cases, whether Nyquist or Bode plots are used, the controller parameters are selected such that specified minimum values of the gain and phase margins are obtained. The gain and phase margins are defined in section 5.3 below.

The closed loop frequency domain method involves the direct optimization of the closed loop frequency response. Such a response is continuously modified by systematically changing the controller parameters until a response with desirable characteristics is obtained.

5.2.3 Root locus (s-domain) method

The root locus is a plot, in the complex plane, of the roots of the characterisctic equation of the closed loop system as a function of the proportional gain of the controller. This plot is easily constructed using a simple set of rules such as the fact that the loci of the closed loop poles start from the locations of the open loop poles where the controller gain is zero and finish at the locations of the open loop zeros or infinity where the controller gain is infinity. One disadvantage of the root locus method is that it is difficult to apply to systems containing time delays. More details concerning this and the frequency response methods can be found in most textbooks on process control such as the book by Coughanowr and Koppel [1965].

Compared to the time domain approaches, the root locus and frequency domain methods have the advantage of offering much more insight into the structure of the system being analysed or designed. However, they suffer from the fact that, in general, one can not make an accurate guess of their equivalent time domain closed loop responses. In addition these methods can not handle system constraints directly.

5.3 Controller Design Criteria

5.3.1 Time domain criteria

When designing single loop control systems, figure 5.1, in the time domain, the goodness of the closed loop dynamic behaviour is normally judged by certain attributes of the system response to a step change in the set point. These criteria are defined as follows:

5.3.1.1 Steady state error, $e(\infty)$:

$$e(\infty) = \lim_{t \to \infty} e(t) \tag{5.1}$$

For the case where the plant or the controller contains an integrator, the steady state error is always zero.

5.3.1.2 Rise time, t_1:

The rise time is given as the solution of the following problem:

$$\min \{t : y(t) = 0.9y(\infty);\ 0 \leqslant t < \infty\} \tag{5.2}$$

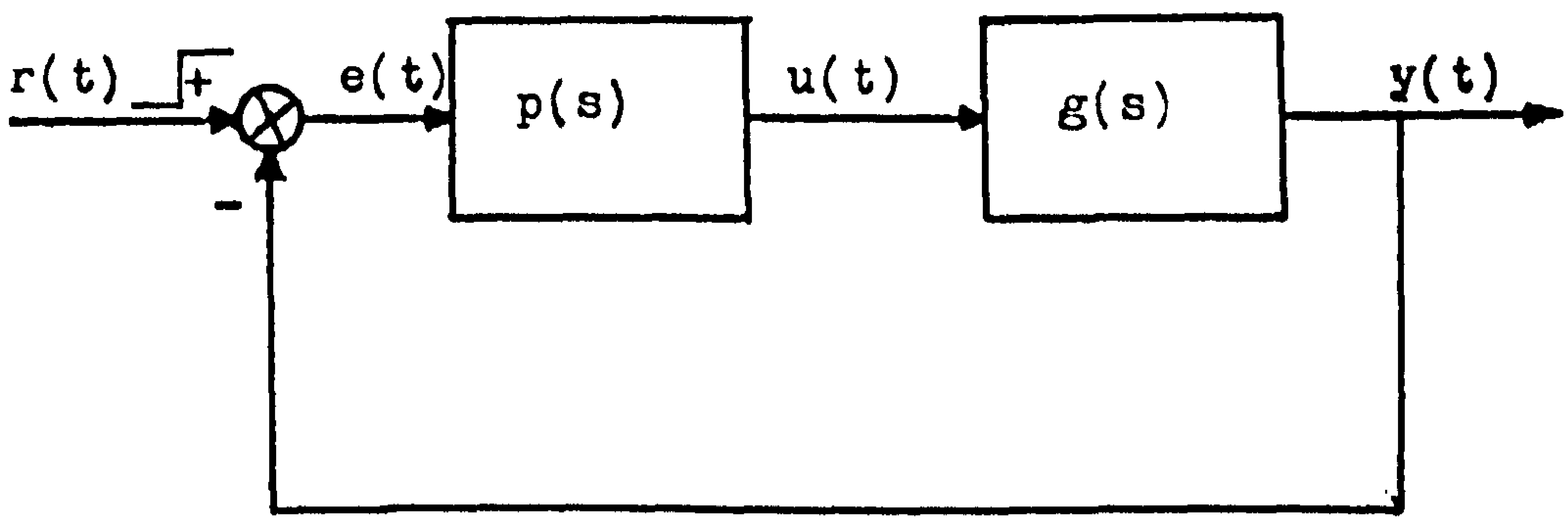


Figure 5.1 SISO feedback control loop

5.3.1.3 Overshoot, m_p:

The overshoot is defined as:

$$m_p = \begin{cases} \dfrac{y_{max}-y(\infty)}{y(\infty)} & \text{if } y_{max}>y(\infty) \\ 0 & \text{if } y_{max}\leqslant y(\infty) \end{cases} \qquad (5.3)$$

where,

$$y_{max} = \max \{y(t):0\leqslant t<\infty\} \qquad (5.4)$$

5.3.1.4 Settling time, t_2:

The settling time, t_2, is given as the solution of:

$$\max \{t:|e(t)|\geqslant 0.02|y(\infty)|;\ 0\leqslant t<\infty\} \qquad (5.5)$$

5.3.1.5 Maximum controller output, $|u|_{max}$:

Another important criterion is the control effort required to achieve a certain system performance. The maximum controller output, $|u|_{max}$, is a measure of the likelihood of controller saturation and hence performance deterioration. It is given by:

$$|u|_{max} = \max \{|u(t)|:0\leqslant t<\infty\} \qquad (5.6)$$

5.3.2 Frequency domain criteria:

In the frequency domain there are many conflicting and nonconflicting criteria which can be used for computerised controller design. Some of the widely used objectives are the open loop Phase (PM) and Gain (GM) margins, and the closed loop peak ratio (M_r) and reasonant frequency (w_r).The PM and GM indicate the degree of system stability, w_r is related to the speed at which the time response settles and M_r indicates how oscillatory is this time response.

5.3.2.1 Reasonant peak ratio, M_r, and reasonant frequency, w_r:

M_r and w_r are obtained through solving the following problem:

$$\min_{w} \{-|CLTF(wj)|\} \tag{5.7}$$

where the closed loop transfer function, CLTF(s), is given by:

$$CLTF(s) = \frac{p(s)g(s)}{1+p(s)g(s)} \tag{5.8}$$

where j is the imaginary unit, $j=\sqrt{-1}$.

The solution of problem (5.7) is w_r. M_r is defined as:

$$M_r = |CLTF(w_r j)| \tag{5.9}$$

5.3.2.2 Phase (PM) and Gain (GM) margins:

The PM is given by:

$$PM = 180^{o} + \angle OLTF(w_p j) \tag{5.10}$$

where w_p is the solution of :

$$\max_{w} \{w: |OLTF(wj)| = 1\} \tag{5.11}$$

and the Open Loop Transfer Function, OLTF(s), is:

$$OLTF(s) = p(s)g(s) \tag{5.12}$$

Similarly the gain margin is given by:

$$GM = \frac{1}{|OLTF(w_{co})|} \tag{5.13}$$

where the crossover frequency, w_{co}, is the solution of:

$$\max_{w} \{w: \angle OLTF(wj) = -180^{o}\} \tag{5.14}$$

5.4 Application of the Proposed Design Algorithm to the Design of SISO Controllers

Here, the algorithm proposed in section 3.2, for solving a problem for which the aim is to minimize a vector of criteria rather than a scalar index, is applied to the design of SISO controllers. The design criteria can be attributes of the time response of the controlled plant or frequency domain objectives or, if desired, a combination of the two. In this work, we will concentrate on the use of the time domain criteria only.

Since the design algorithm involves the solution of a series of constrained optimization problems, a computer program, which uses the Hooke and Jeeves(HJ) method, described in chapter 4, has been written for such a purpose and it is given in the software appendix at the end of this thesis. A subroutine which caters for the simulation of time delays is also provided. This program is selfcontained and it is very easy to use. All that is required from the user is to define his system and the design criteria. This is a simple enough matter since the main aim of the ISIM language in which the program is written, is to relieve the user from the difficulties involved in such activities.

5.4.1 Example 1: Third Order Plant

Consider the plant:

$$g(s) = \frac{10}{s(s+1)(s+5)} \tag{5.15}$$

for which the controller:

$$p(s) = \frac{p_1(1+p_2 s)}{1+p_2 p_3 s} \tag{5.16}$$

has been designed by D'Azzo and Houpis [1966] using the root locus method, and by Zakian and Al-Naib [1973] who used the method of inequalities.

This same controller is used in this work. It is assumed that a settling time equal to 2.5 is deemed satisfactory and that controller saturation is unlikely to occur. Hence, both, the maximum controller output and the settling time are considered as secondary criteria with the latter included in the design problem as a hard constraint. The rise time, t_1, and the overshoot, m_p, are the primary criteria. This example and the ones to follow are all assumed to be based on dimensionless time.

The achievable minimum value of the rise time is obtained by solving the problem:

$$\min \{t_1 : t_2 < 2.5;\ m_p < 0.4;\ P_L \leqslant P \leqslant P^U\} \tag{5.17}$$

where a closed loop response with an overshoot of 40% or more is considered to be undesirable. $P_L=[p_{iL}]$ $(i=1,2,3)$ and $P^U=[p_i^U]$ $(i=1,2,3)$. Where subscript L and superscript U denote, respectively, the lower and upper bounds on the design variables (controller parameters). We have used the bounds given by Zakian and Al-Naib [1973], i.e $P_L=(0.01,0,0.01)$ and $P^U=(100,20,10)$. Problem (5.17) yields:

$P = (2.592, 1.675, 0.024)$; $t_1=0.3$; $t_2=2.25$; $m_p=0.4$ and $|u|_{max}=108.0$.

If the rise time is unbounded, closed loop system responses with zero overshoot, which is the minimum value, can be obtained by a large number of controller designs. One of these solutions, however, is the second extreme nondominated solution. Such a design can be obtained by solving the following problem:

$$\min \{ t_1 : t_2 < 2.5;\ m_p \leq 0;\ P_L \leq P < P^U \} \tag{5.18}$$

which yields:

$P = (0.864, 1.297, 0.034)$; $t_1=0.95$; $t_2=1.2$; $m_p=0.0$; and $|u|_{max}=25.4$.

The nondominated set of solutions is shown in figure 5.2 and table 5.2. These solutions may be obtained by minimizing the rise time for different values of the overshoot between 0 and 0.4 or optimizing the overshoot for different values of the rise time between 0.3 and 0.95. Since the rise time must be an integral value of the integration step length the second approach has been followed. Clearly, depending on the application in question, anyone of the nondominated solutions can be chosen as the best design. However, in most cases the

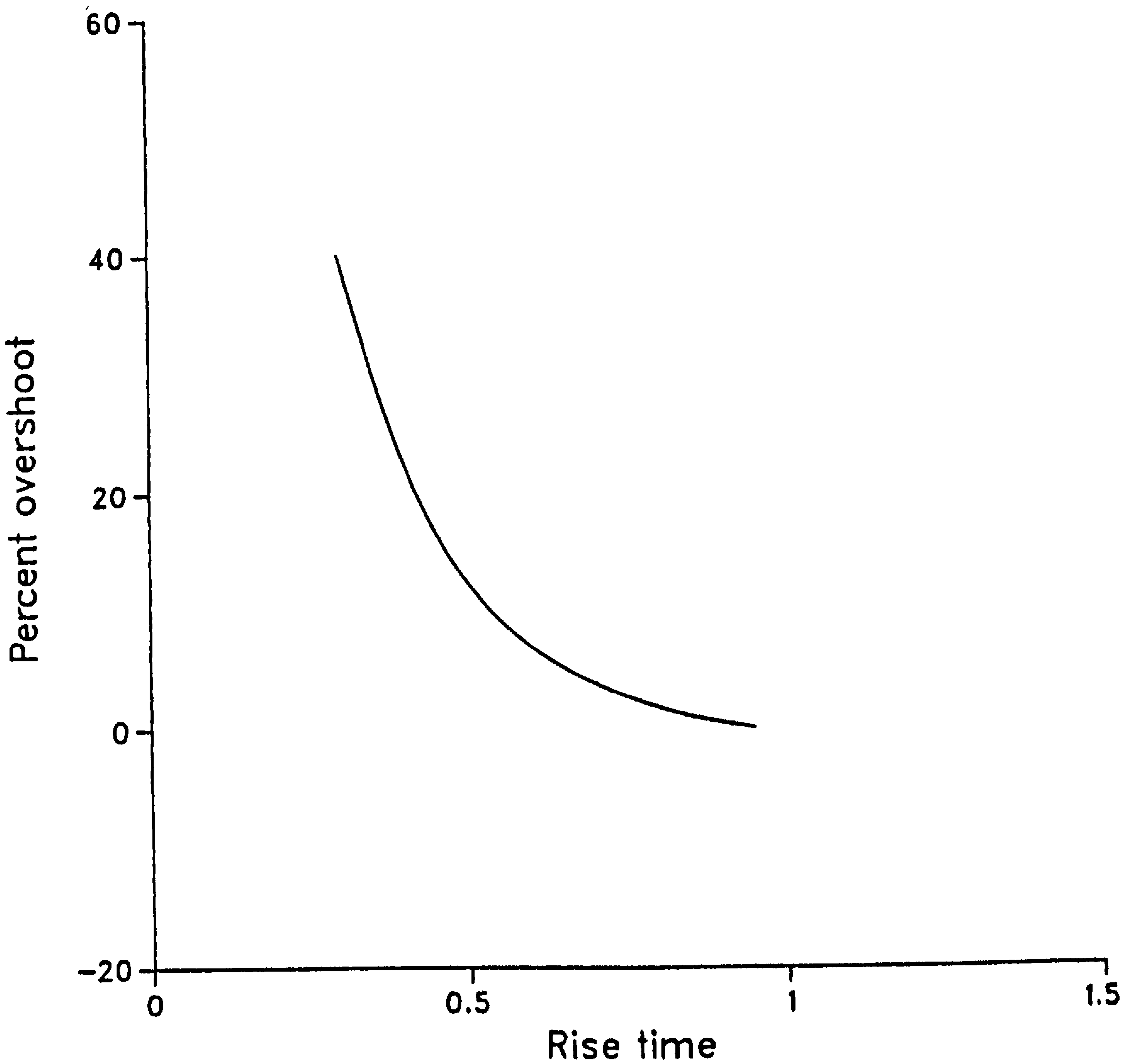


Figure 5.2 Nondominated set.

designer can eliminate a large number of these noninferior solutions without resorting to his other quantifiable and subjective criteria. Let us divide the nondominated set to three regions as follows:

region I : $0.7<t_1\leqslant 0.95$

region II : $0.4<t_1\leqslant 0.7$

region III : $0.3\leqslant t_1\leqslant 0.4$

In region I significant improvements can be obtained in the rise time at the expense of small increases in the overshoot. An increase of 3.8% in the overshoot results in

Table 5.2: A set of nondominated solutions

solution P	t_1	m_p	t_2	$\|u\|_{max}$
S1 (2.592,1.675,0.024)	0.3	0.400	2.25	108.0
S2 (1.826,1.592,0.026)	0.4	0.228	1.70	70.2
S3 (1.330,1.655,0.026)	0.5	0.125	2.15	51.2
S4 (1.072,1.324,0.032)	0.7	0.038	2.50	33.5
S5 (0.944,1.197,0.033)	0.85	0.011	2.50	29.5
S6 (0.864,1.297,0.034)	0.95	0.000	1.20	25.4

0.25 (from 216.7% over the minimum (0.3) to 133.3% over the minimum) reduction in the rise time. In most cases such tradeoffs are accepted and region I eliminated from further consideration. In region III, the overshoot is reduced from 40% to 22.8% for a mere 33% increase over the minimum value of the rise time. Also notice the large reduction in the maximum controller output in this region. Again, such tradeoffs are usually accepted and this region is eliminated as well.

Now, only those designs belonging to region II remain as candidates for the best solution. At this stage secondary and subjective criteria may be heavily relied on in the choice of this best design. Assume that due to the high reduction in the maximum controller output the solution with 0.7 rise time (S4) is chosen as the final design. In table 5.3, this solution is compared with those obtained by Zakian and Al-Naib [1973], and D'Azzo and Houpis [1966]. The solution which yields the minimum value of the ISE is also given in this table. The closed loop time responses are shown in figure 5.3, in which it can be clearly seen that the time response of the S4 design is better than those of the other designs.

A nondominated solution located in region III has been obtained by ZA. Normally this is not to be expected since the aim of the moving boundaries approach is to find any solution which satisfies the problem constraints. As the

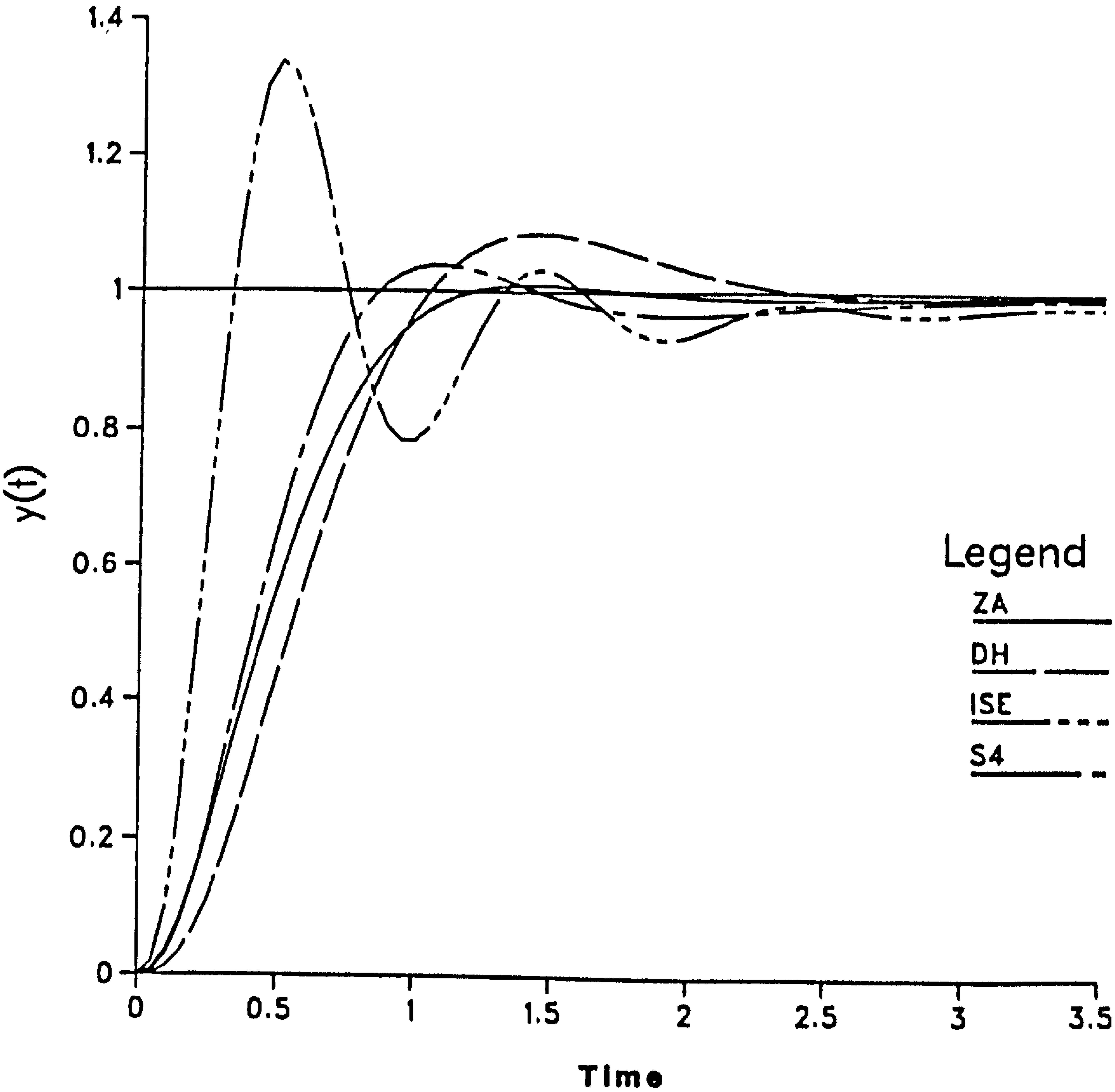


Figure 5.3

set of feasible solutions is usually very large compared to its constituent pareto optimal Subset, in most cases, it is improbable for the method of inequalities to locate one of the nondominated solutions.

To confirm the claim that the use of a fuzzy overall performance index may lead to misleading results, the ISE value achieved by every design is also included in table 5.3. Had this index been used to compare the different designs then the solution of DH would have been considered highly undesirable as it results in an increase of 110.4% over the achievable minimum value. Yet, except for the rise time, the DH design outperforms the solution which yields the minimum ISE value in all the design criteria.

Table 5.3: Comparison of results

design P	t_1	m_p	t_2	$\lvert u \rvert_{max}$	ISE
Zakian and Al-Naib (ZA) (0.997,1.119,0.0125)	0.9	0.009	1.1	79.8	0.339
D´Azzo and Houpis (DH) (1.0,1.0,0.1)	0.9	0.084	2.2	10.0	0.423
Minimum ISE (MISE) (1.562,3.146,0.013)	0.3	0.336	3.2	121.1	0.201
S4 (1.072,1.324,0.032)	0.7	0.038	2.5	33.5	0.314

5.4.2 Example 2: Second Order Plant with Delay

Edgar et al. [1981] used a frequency based interactive computer package to design an ideal PID controller for a plant with the transfer function:

$$g(s) = \frac{\exp(-s)}{(10s+1)(5s+1)} \tag{5.19}$$

Recently, Harris and Mellichamp [1985] designed the same controller using a conventional optimization approach. A weighted sum of the reasonant peak ratio M_r, the Phase Margin (PM) and the reasonant frequency, w_r, was used as the objective function. They assumed arbitrary values for the weighting factors and claimed that these values need not be varied from case to case. Here, a practical controller which has the transfer function:

$$p(s) = p_1\left(\frac{1}{p_2 s} + \frac{1+p_3 s}{1+ \alpha p_3 s}\right) \tag{5.20}$$

is employed.

The parameter α is chosen to be small, (α=0.1), so that the results of the different approaches can be compared without much distortion.

Following the work of Ziegler and Nichols [1942], a fixed ratio of 4 between the integral time and the derivative time, p_2/p_3, was assumed by Harris and Mellichamp. This ratio has also been used in this work.

The nondominated set of solutions is given in figure 5.4 and table 5.4 where t_1 and m_p have been chosen as the primary criteria. Any design whose settling time or overshoot exceeded values of 15 and 40%, respectively, has been deemed unsatisfactory.

After analysing the nondominated set, assume that the designer selects the solution with a rise time of 3.5 (S3) as his best design. Table 5.5 compares this solution with designs obtained using other approaches. The time response of some of these designs are also shown in figure 5.5.

The RMS approach refers to the minimum IAE tuning relationships proposed by Rovira et al. [1969]. This method, however, requires the presence of an approximate FOPDT

Table 5.4: A set of nondominated solutions

solution P	t_1	m_p	t_2	$\|u\|_{max}$
S1 (11.36,10.144,2.536)	2.75	0.403	14.1	114.0
S2 (8.56,13.260,3.315)	3.00	0.262	13.5	85.6
S3 (6.68,14.038,3.508)	3.50	0.125	7.7	66.8
S4 (5.33,15.968,3.992)	4.00	0.041	12.0	53.3
S5 (4.79,15.912,3.978)	4.50	0.000	15.0	47.9

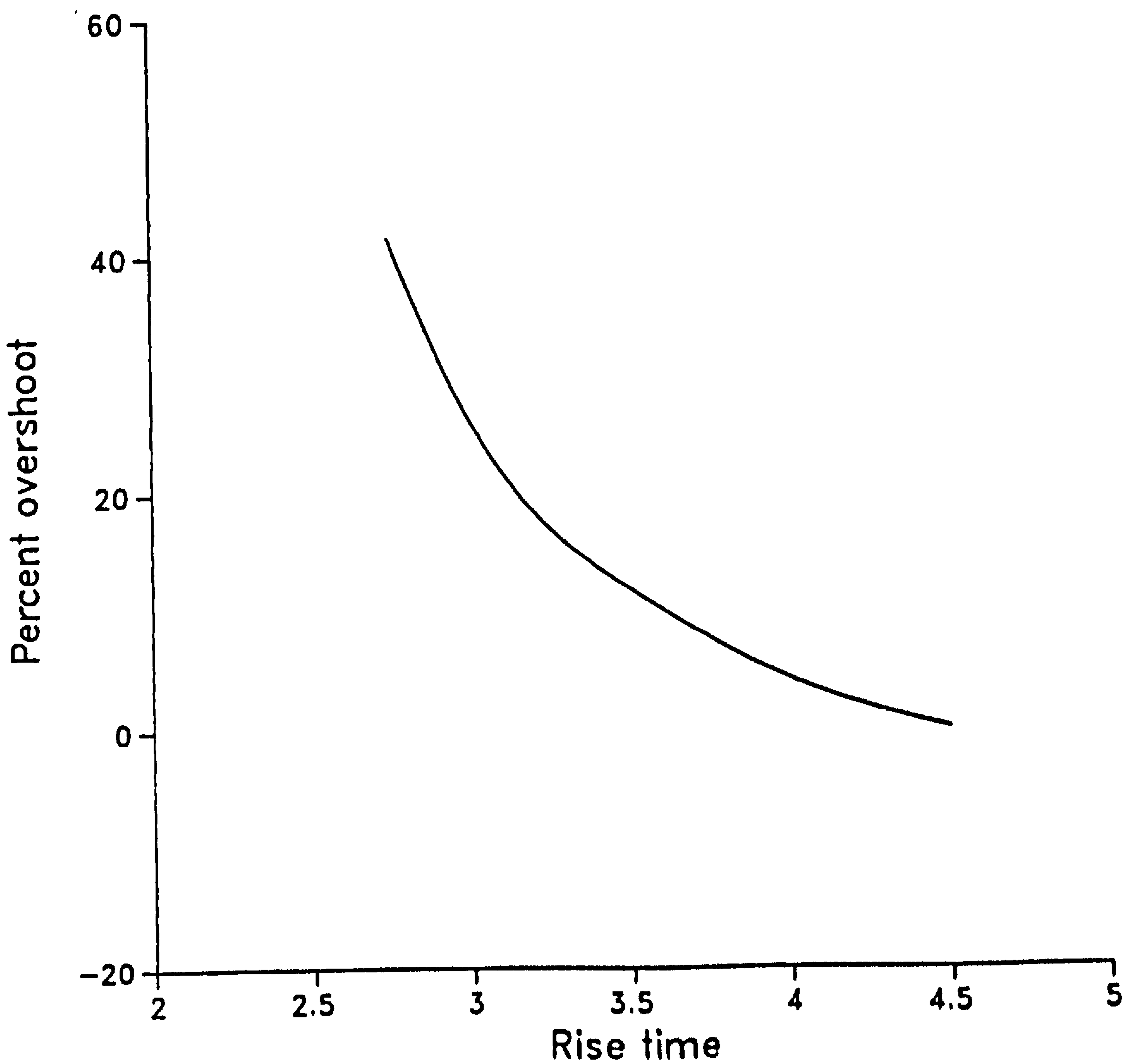


Figure 5.4 Nondominated set.

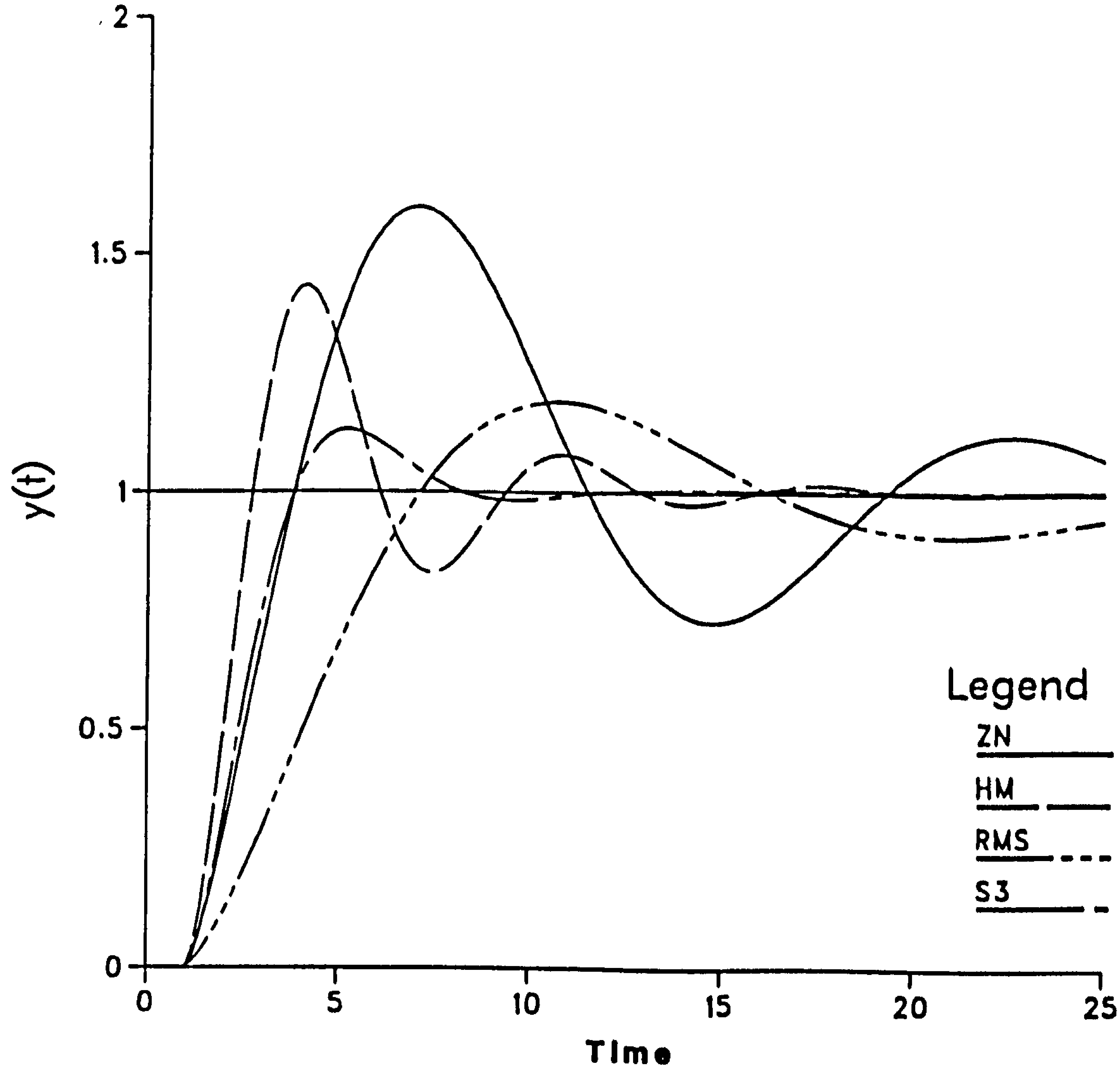


Figure 5.5

model of the plant. Using the reaction curve procedure of Miller et al [1967], fit 2, the plant transfer function, equation (5.19), reduces to:

$$g(s) = \frac{\exp(-2.6s)}{14.2s + 1} \tag{5.21}$$

Hougen [1979] proposed tuning relationships which are based on the frequency response of SOPDT plants and practical controllers of the form given by equation (5.20).

Table 5.5: Comparison of results

design P	t_1	m_p	t_2	$\lvert u \rvert_{max}$
Ziegler and Nichols (ZN) (9.44,5.83,1.46)	3.60	0.588	33.6	94.4
Harris and Mellichamp (HM) (9.44,12.56,3.39)	2.60	0.420	14.0	107.0
Edgar Heeb and Hougen (EHH) (9.44,9.0,4.0)	2.62	0.420	19.0	94.4
Hougen (6.50,10.0,3.68)	3.72	0.145	19.5	65.0
Rovira Murrill and Smith (RMS) (4.75,19.83,1.05)	6.45	0.190	28.0	47.5
S3 (6.68,14.04,3.51)	3.50	0.125	7.7	66.8

This is the main reason why the controller obtained using his approach appears to give better performance than the majority of the designs in table 5.5. Still, despite the restriction imposed on the design variables, i.e $p_2/p_3=4$, the superiority of solution S3 is quite apparent.

5.4.3 Example 3: Fifth Order Plant

Consider the plant:

$$g(s) = 1/(s+1)^5 \tag{5.22}$$

which can be approximated by the FOPDT model:

$$g(s) = \frac{\exp(-2s)}{3.42s+1} \tag{5.23}$$

The design of a PI controller for this plant is here considered. The a priori specifications include constraints on the controller output and the settling time which are not to exceed values of 1.5 and 25 respectively. the overshoot and the rise time are again chosen to be the primary criteria.

Following the same approach used in example 1, the generated nondominated set is given in table 5.6 and shown in figure 5.6. Assume that the noninferior solution with a rise time of 6.6 (S4) is selected as the best design. Table 5.7 compares this design with those obtained using the continuous cycling procedure of ZN and the minimum IAE approach of RMS. Their time responses are shown in figure 5.7. It is obvious that design S4 exhibits better performance than the other designs given in this figure.

Table 5.6: A set of nondominated solutions

solution	t_1	m_p	t_2	$\|u\|_{max}$
S1 (0.945,4.313)	6.0	0.121	18.2	1.38
S2 (0.928,4.636)	6.2	0.075	18.8	1.32
S3 (0.898,4.710)	6.4	0.048	19.0	1.28
S4 (0.864,4.700)	6.6	0.026	19.4	1.24
S5 (0.839,4.700)	6.8	0.009	20.0	1.20

Table 5.7: Comparision of results

design	t_1	m_p	t_2	$\|u\|_{max}$
ZN P=(1.32,7.20)	5.25	0.132	35.5	1.58
RMS P=(1.20,4.11)	5.12	0.310	32.5	1.73
S4 P=(0.864,4.70)	6.60	0.026	19.4	1.24

5.5 Discussion

The aim of this chapter has been to illustrate the application of the proposed multiobjective design approach to the design of SISO controllers. Usually, the rise time, the settling time, the overshoot and the maximum controller output are the criteria by which a system performance is judged. Here, these attributes have been considered explicitly rather than implicitly as is done with the available single performance index techniques such as the integral of some function of the error or quarter decay ratio approaches. When such techniques are used, no clear cut information is known about the expected controller performance until the design process is finished and the system response is simulated. The achieved performance may or may not be acceptable and it varies considerably from

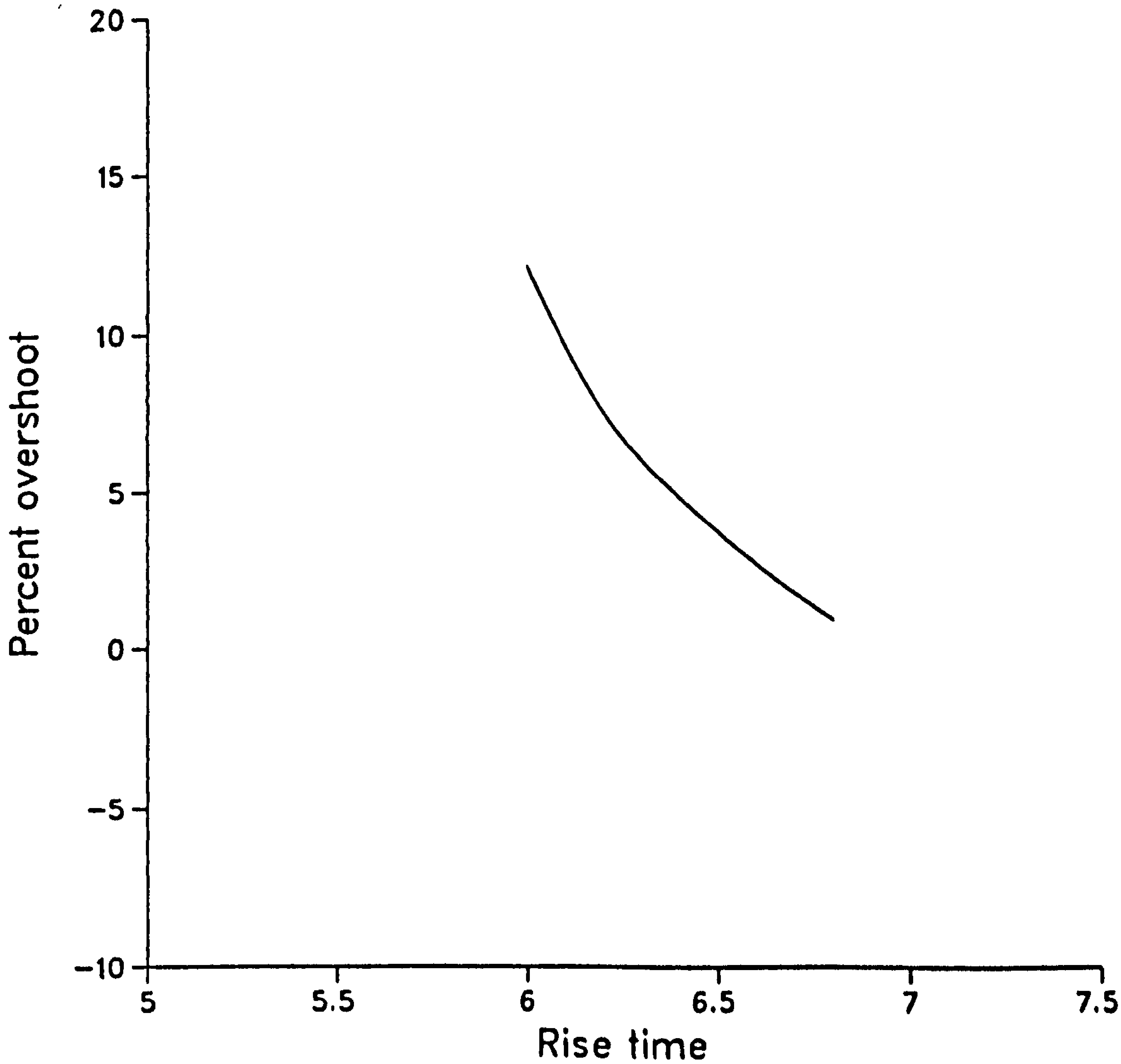


Figure 5.6 Nondominated set.

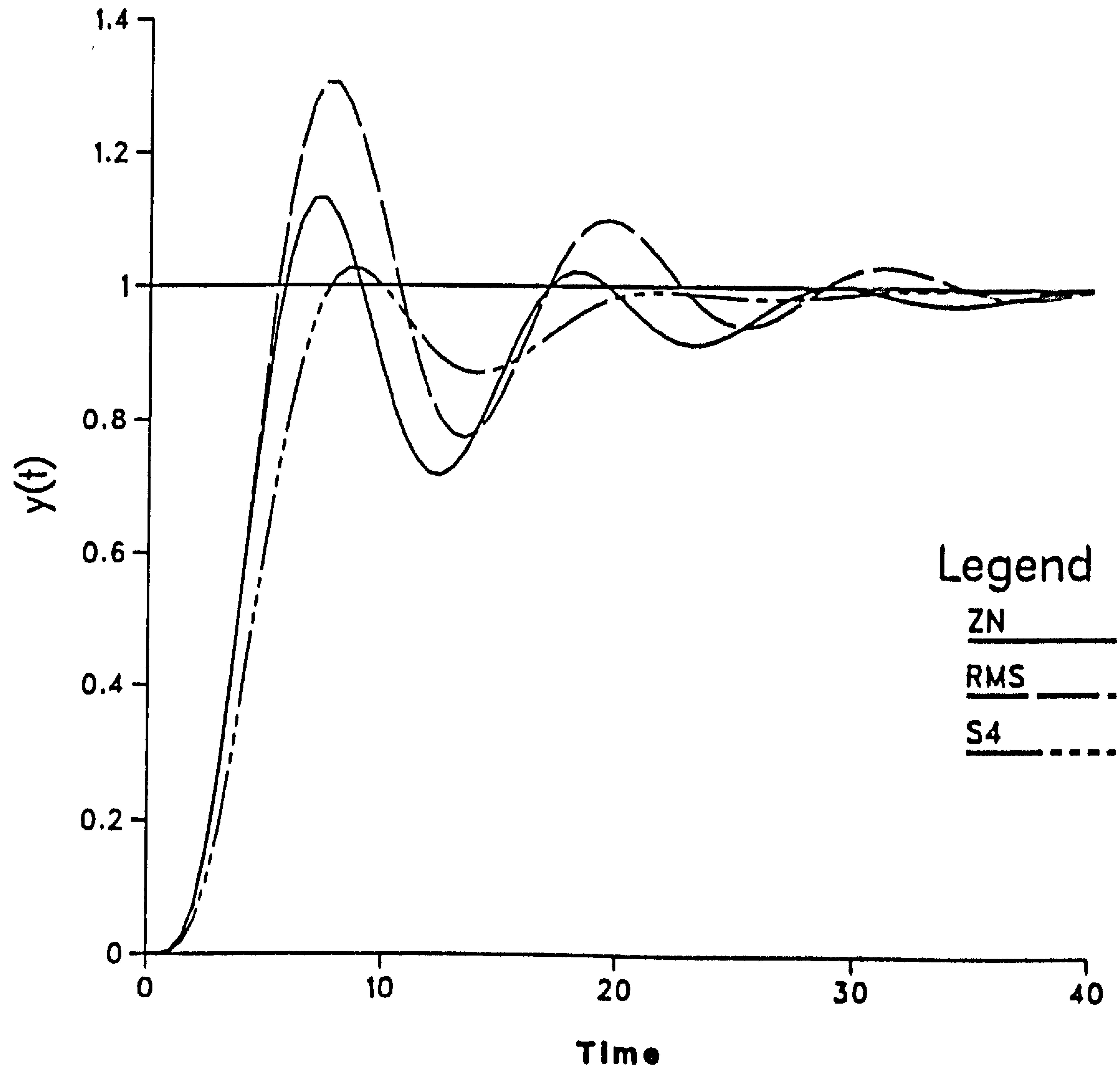


Figure 5.7

case to case. At the problem formulation stage only fuzzy information is available such as the fact that if the ISE is used as the overall performance index then the rise time is heavily weighted and the obtained system is expected to exhibit high overshoot.

The method of inequalities proposed by Zakian and Al-Naib [1973] is one approach where the controller design criteria are considered explicitly. This method however relies on the availability of all the information concerning the sought best design before the design process is started. However, the designer can confidently choose the best solution only if he has at his disposal a clear idea about the achievable solutions and the tradeoffs involved. The method used here provides the designer with such information before he is asked to express his preferences. The examples clearly illustrate the superiority of this approach over the other techniques.

In all the treated examples, the controller structure has been assumed to be fixed, and the rise time and the overshoot have been used as the primary criteria. However, depending on the particular problem at hand the designer can select any combination of criteria as his set of primary objectives, and if at any stage of the design process he feels unhappy about the controller structure, he can choose a different structure of higher complexity and start all over again.

Appendix 5A

The controller tuning relationships used in the examples treated in chapter 5 are given here.

(a) Ziegler and Nichols [1942]:

PI controller, $p(s)=p_1(1+s/p_2)$:

$$p_1 = 0.45k_u$$

$$p_2 = p_u/1.2$$

PID controller, $p(s)=p_1(1+s/p_2+p_3s)$:

$$p_1 = 0.6k_u$$

$$p_2 = p_u/2$$

$$p_3 = p_u/8$$

where k_u and p_u are, respectively, the ultimate gain and the ultimate period. p_1, p_2 and p_3 are the controller proportional gain, reset time and derivative time respectively.

(b) Rovira et al. [1969] IAE relationships:

PI controller:

$$k_p p_1 = 0.758(R)^{-0.861}$$

$$T/p_2 = 1.02 - 0.323R$$

PID controller:

$$k_p p_1 = 1.086(R)^{-0.869}$$

$$T/p_2 = 0.740 - 0.130R$$

$$p_3/T = 0.348(R)^{0.914}$$

where $R=T_d/T$. k_p, T_d and T are the plant steady state gain, time delay and time constant respectively.

(c) Hougen [1979] tuning relationships for a compensator of the form given by equation (5.20) with $\alpha=0.1$, controlling a SOPDT plant:

$$k_p p_1 = \frac{0.8T_1^{0.7}T_2^{0.3}}{T_d}$$

$$p_2 = 0.5T_1 + T_2$$

$$p_3 = 0.1(T_d T_1 T_2)^{1/3}$$

where T_1 and T_2 are, respectively, the smallest and largest plant time constants.

For the interested reader, table 5A below gives references to some of the available time-domain, open loop methods for tuning ideal controllers.

Table 5A Some of the available controller tuning methods.

Method	step test	performance index	plant model
a	SP	1/4 decay ratio	FOPDT
b	LD	ISE, IAE & ITAE	FOPDT
c	LD	ITAE	SOPDT
d	SP	1/4 decay ratio	FOPDT
e	SP	IAE & ITAE	FOPDT
f	SP	ISE	FOPDT

SP = set point

LD = load disturbance

a -- Cohen and Coon [1942]

b -- Lopez et al. [1967]

c -- Lopez et al. [1969]

d -- Smith et al. [1966]

e -- Rovira et al. [1969]

f -- Morari et al. [1984]

CHAPTER 6

INTEGRATED DESIGN AND CONTROL OF A CSTR

6.1 Introduction

In this chapter, the integrated design of a hypothetical case study is considered. The process is a Continuous Stirred Tank Reactor (CSTR) in which an exothermic first order irreversible reaction ($A \rightarrow B$) takes place, figure 6.1. The additional heat required to sustain the reaction is supplied by a heating coil. This example, though simple, retains the basic features of many practical processes.

A chemical reactor has been chosen as a case study for the following reasons:

(a) It is one of the most common unit operation in the chemical and petrochemical industries.

(b) It is known to exhibit stability and control problems.

(b) Downstream of the reactor there usually lies a distillation column; The operation of which is highly influenced by variations in its feed characteristics and hence the controllability of the reactor.

During the years, the stability and open loop dynamic behaviour of chemical reactors have been the subject of a large number of studies which are selectively reviewed by

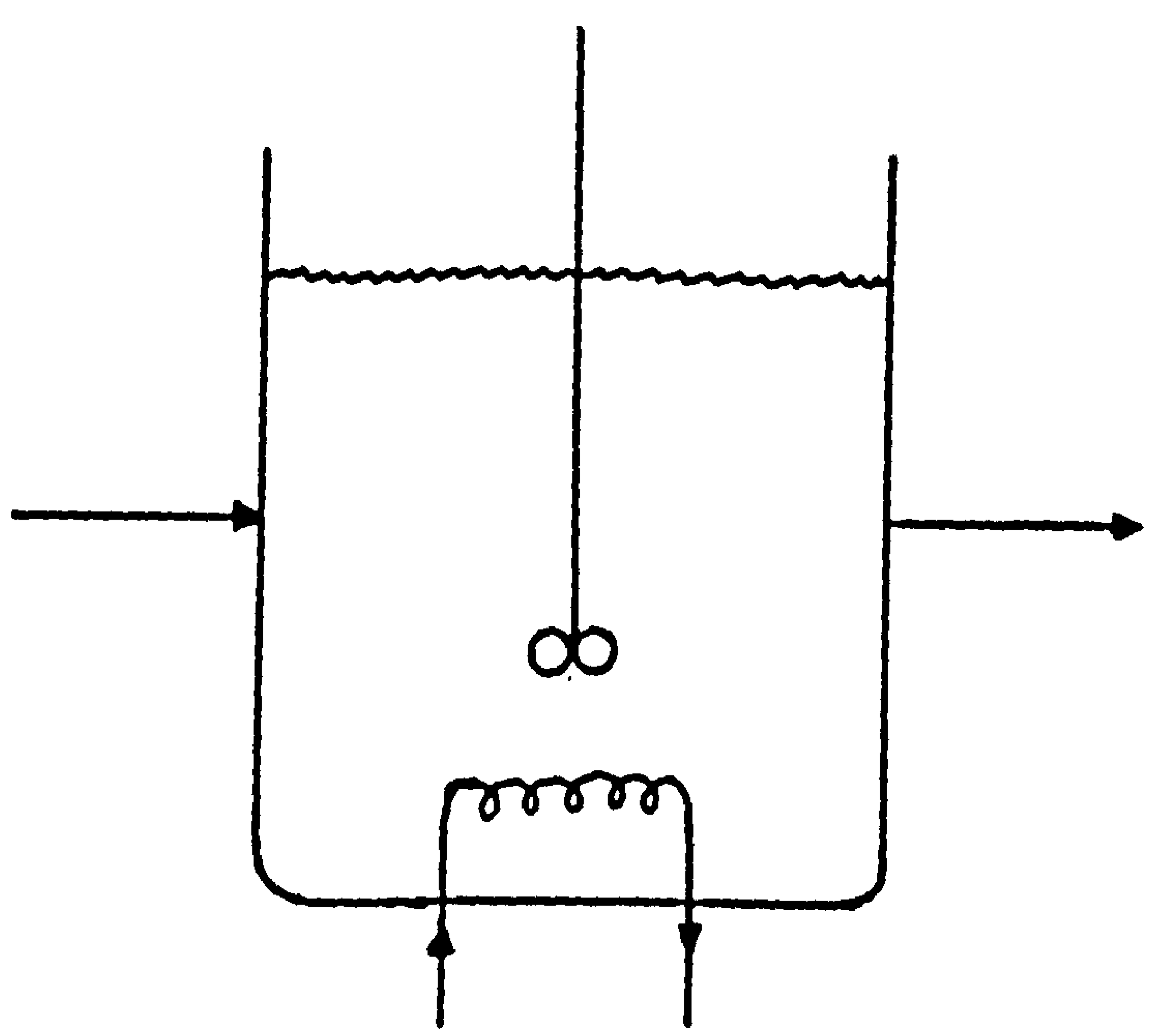


Figure 6.1

Uppal et al. [1974]. A number of approaches have been employed for analysing the stability of CSTR's which include the phase plane, pioneered by Aris and Amundson [1958], the Liapunov's techniques and the circle criterion.

The control of CSTR systems has also been considered by a considerable number of workers. A brief review of the studies carried out before 1973 can be found in the book on "Chemical Reactor Theory" by Lapidus and Amundson [1977]. The CSTR continue to be a good example for demonstrating new control algorithms. Some of the recent studies include the application of bang-bang control to a CSTR by Bruns and Bailey [1977] who used the cooling fluid rate as the manipulated variable to control the reactor temperature, and the design of (2x2) multivariable controllers by Taiwo [1979] using the Method of Inequalities. In the latter study, the feed flow rate and the heating fluid rate have been employed as the manipulated variables to control the reactor temperature and concentration.

The chapter is structured as follows. The steady state, and general linear and nonlinear dynamic models of the reactor are presented in sections 2 and 3 respectively. In section 4 the usual steady state profit maximization design procedure is carried out, and the open loop dynamic behaviour of the obtained optimum design is examined in section 5.

The reactor can be controlled using one of a large number of possible control systems. For example, the possible manipulated variable(s) include the feed temperature, concentration and flow rate, and the heating fluid flow rate and inlet temperature. Two of the possible controlled variable(s) are the reactant concentration and temperature. Compensators of varying degrees of complexity can be employed such as conventional SISO PID controllers, full-blown multivarible PID controllers in which every input affects every output and self-tuners.

Two simple systems, referred to as system 1 and system 2, are considered in this study. In system 1 the plant is controlled using a SISO PI controller with the heating fluid flow rate as the manipulated variable controlling the reactor temperature. In system 2 the CSTR temperature and concentration are simultaneously controlled by manipulating the feed and heating fluid flow rates, and the controller is designed using the LQ Problem formulation. Sections 6 and 7 are, respectively, concerned with the integrated design and control of systems 1 and 2.

6.2 Steady state model

The steady state equations describing the reactor are:

Production rate:

$$G_p = F(C_{af}-C_a) \tag{6.1}$$

Material balance on A:

$$F(C_{af}-C_a) - kVC_a = 0 \tag{6.2}$$

Reaction rate constant, k:

$$k = k_o \exp\{-E_a/(R_g T)\} \tag{6.3}$$

Overall energy balance:

$$F C_p e (T_f - T) + (-\Delta H) k V C_a + Q_h = 0 \tag{6.4}$$

Energy balance for the heating fluid:

$$Q_h = F_h C_{ph} e_h (T_h - T_o) \tag{6.5}$$

Heat transfer between the coil and the reactor:

$$Q_h = U_c A_h (T_{av} - T) \tag{6.6}$$

where,

$$T_{av} = (T_h + T_o)/2 \tag{6.7}$$

In equation (6.6) the temperature driving force is represented by the arithmetic mean instead of the log-mean temperature.

The following symbols have been used:

G_p production rate, Kmole/hr

F feed rate, m^3/hr

C_p heat capacity of the feed, Kj/(kg)(^oK)

ϱ_g density of the feed, kg/m^3

C_{af} feed concentration, $Kmole/m^3$

C_a concentration of the reactant in the stream leaving the reactor, $Kmole/m^3$

V reactor volume, m^3

k reaction rate constant, hr^{-1}

k_o frequency factor, hr^{-1}

E_a activation energy, Kj/Kmole

R_g gas constant, Kj/(Kmole)(^oK)

T reactor temperature, ^oK

$(-\Delta H)$ heat of reaction, Kj/(Kmole of A)

Q_h heat duty supplied by the coil, Kj/hr

F_h heating fluid rate, m^3/hr

C_{ph} heat capacity of the heating fluid, Kj/(kg)(^oK)

ϱ_h density of the heating fluid, kg/m^3

T_h inlet temperature of the heating fluid, ^oK

T_o outlet temperature of the heating fluid, ^oK

U_c overall heat transfer coefficient, Kj/(hr)(^oK)(m^2)

A_h heat transfer area of the coil, m^2

T_{av} average temperature of the heating liquid, ^oK.

6.3 Dynamic Models

The reactor unsteady mass and energy balances are:

$$\frac{dC_a}{dt} = \frac{F}{V}(C_{af}-C_a) - kC_a \tag{6.8}$$

$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \frac{(-\Delta H)}{C_p e} k C_a$$

$$+ \frac{U_c A_h L F_h}{V C_p e (1 + L F_h)} (T_h - T) \qquad (6.9)$$

where,

$$L = \frac{2 C_{ph} e_h}{U_c A_h} \qquad (6.9a)$$

The detailed development of the above model can be found in chapter 3 of the book by Douglas [1972]. The assumptions required for its derivation include:

(a) The reactor is perfectly mixed

(b) The dynamics of the heat exchanger (coil) are negligible

(c) The temperature driving force is based on the average temperature of the coil

(d) The physical properties, which include the densities, the heat capacities of the feed and heating fluid as well as the reaction rate parameters, are constant.

6.3.1 Linear model

Consider the case where F, C_{af}, T_f, F_h and T_h vary from their steady state values which cause C_a and T to deviate, then linearisation of equations (6.8) and (6.9) give in terms of the perturbation variables:

$$\frac{dC_a^*}{dt} = -\left(\frac{F_s}{V} + k_s\right)C_a^* - \frac{E_a k_s C_{as}}{R_g T_s^2}T^* + \frac{C_{afs} - C_{as}}{V}F^* + \frac{F_s}{V}C_{af}^* \qquad (6.10)$$

$$\frac{dT^*}{dt} = \frac{(-\Delta H)k_s}{C_p e}C_a^* - \left[\frac{F_s}{V} - \frac{(-\Delta H)E_a k_s C_{as}}{C_p e R_g T_s^2} + \frac{U_c A_h L F_{hs}}{VC_p e(1+LF_{hs})}\right]T^* + \frac{F_s}{V}T_f^* + \frac{(T_{fs}-T_s)}{V}F^* + \frac{U_c A_h L F_{hs}}{VC_p e(1+LF_{hs})}T_h^* + \frac{U_c A_h L(T_{hs}-T_s)}{VC_p e(1+LF_{hs})^2}F_h^* \qquad (6.11)$$

where the astrisk denotes a deviation variable, e.g $T^* = T - T_s$, and subscript s is used in this section to denote the steady state operating point of interest.

By introducing the dimensionless variables:

$$z_1 = \frac{C_a}{C_{afs}}, \quad z_2 = \frac{C_p e T}{(-\Delta H)C_{afs}}, \quad m_1 = \frac{F}{F_s},$$

$$m_2 = \frac{F_h}{F_{hs}}, \quad m_3 = \frac{C_{af}}{C_{afs}}, \quad m_4 = \frac{C_p e T_f}{(-\Delta H) C_{afs}},$$

$$m_5 = \frac{C_p e T_h}{(-\Delta H) C_{afs}}, \qquad \tau = \frac{F_s t}{V}$$

we obtain:

$$\frac{dx_1}{d\tau} = a_{11}x_1 + a_{12}x_2 + b_{11}u_1 + b_{13}u_3 \qquad (6.12)$$

$$\frac{dx_2}{d\tau} = a_{21}x_1 + a_{22}x_2 + b_{21}u_1 + b_{22}u_2$$

$$+ b_{24}u_4 + b_{25}u_5 \qquad (6.13)$$

where,

$$x_i = z_i^*$$

$$u_i = m_i^*$$

$$a_{11} = -(1 + \frac{k_s V}{F_s})$$

$$a_{12} = - \frac{E_a C_p e k_s V z_{1s}}{R_g (-\Delta H) C_{afs} F_s z_{2s}^2}$$

$$a_{21} = \frac{k_s V}{F_s}$$

$$a_{22} = -\left[1 - \frac{E_a C_p e k_s V z_{1s}}{R_g(-\Delta H) C_{afs} F_s z_{2s}^2} + \frac{U_c A_h L F_{hs}}{F_s C_p e(1+LF_{hs})}\right]$$

$$b_{11} = 1 - z_{1s}$$

$$b_{12} = b_{14} = b_{15} = b_{23} = 0$$

$$b_{13} = b_{24} = 1$$

$$b_{21} = m_{4s} - z_{2s}$$

$$b_{22} = \frac{U_c A_h L F_{hs}(m_{5s} - z_{2s})}{C_p e(1+LF_{hs})^2 F_s}$$

$$b_{25} = \frac{U_c A_h L F_{hs}}{F_s C_p e(1+LF_{hs})}$$

Equations (6.12) and (6.13) can be written in matrix form as follows:

$$\dot{x} = Ax + B^+u^+ \tag{6.14}$$

where the symbol (.) denotes the differentiation operator $d/d\tau$.

$$A = [a_{ij}] \qquad i=1,2; \quad j=1,2$$

$$B^+ = [b_{ij}] \qquad i=1,2; \quad j=1,2,\ldots,5$$

$$x^T = [x_1, x_2]$$

$$M^T = [m_i] \qquad i=1,2,\ldots,5$$

$$(u^+)^T = [u_i] \qquad i=1,2,\ldots,5$$

where superscript T denotes the transpose matrix.

Taking the Laplace transform of equation (6.14) we obtain:

$$X(s) = G(s)U^+(s) \tag{6.15}$$

where

$$G(s) = (sI-A)^{-1}B^+ \tag{6.16}$$

The (2x5) plant transfer function matrix G(s) has the form:

$$G(s) = [g_{ij}(s)] \quad i=1,2; \quad j=1,2,\ldots,5 \tag{6.17}$$

$$G(s) = \frac{1}{D(s)} \left[\begin{matrix} k_{11}(T_{z1}s+1) & k_{12} \\ k_{21}(T_{z3}s+1) & k_{22}(T_{z4}s+1) \end{matrix} \right.$$

$$\left.\begin{array}{lll} k_{13}(T_{z2}s+1) & k_{14} & k_{15} \\ \\ k_{23} & k_{24}(T_{z4}s+1) & k_{25}(T_{z4}s+1) \end{array}\right] \quad (6.18)$$

where,

$$k_{11} = N(a_{12}b_{21}-a_{22}b_{11})$$

$$T_{z1} = Nb_{22}/k_{11}$$

$$k_{12} = Na_{12}b_{22}$$

$$k_{13} = -\ Na_{22}b_{13}$$

$$T_{z2} = -1/a_{22}$$

$$k_{14} = Na_{12}b_{24}$$

$$k_{15} = Na_{12}b_{25}$$

$$k_{21} = N(b_{11}a_{22}-a_{11}b_{21})$$

$$T_{z3} = Nb_{21}/k_{21}$$

$$k_{22} = -Na_{11}b_{22}$$

$$T_{z4} = -1/a_{11}$$

$$k_{23} = Na_{21}b_{13}$$

$$k_{24} = - Na_{11}b_{24}$$

$$k_{25} = - Na_{11}b_{25}$$

$$N = T_p^2$$

$$T_p = \frac{1}{(a_{11}a_{22}-a_{12}a_{21})^{1/2}}$$

The plant characteristic equation, D(s), is given by:

$$D(s) = T_p^2 s^2 + 2\zeta T_p s + 1 \qquad (6.19)$$

where,

$$\zeta = \frac{-(a_{11}+a_{22})T_p}{2}$$

6.3.2 Nonlinear model

Through manipulation of equations (6.8) and (6.9) we have:

$$\dot{z}_1 = m_1(m_3-z_1) - \alpha z_1 \exp(-\beta/z_2) \tag{6.20}$$

$$\dot{z}_2 = m_1(m_4-z_2) + \alpha z_1 \exp(-\beta/z_2) + \frac{\gamma L m_2}{(1+F_{hs}Lm_2)}(m_5-z_2) \tag{6.21}$$

where,

$$\beta = \frac{E_a C_p e}{R_g(-\Delta H)C_{afs}}$$

$$\alpha = k_o \frac{V}{F_s}$$

$$\gamma = \frac{F_{hs}U_c A_h}{F_s C_p e}$$

6.4 Maximum profit design

The rate of profit return, P_r, from the reaction system shown in figure 6.1 can be written as:

$$P_r = B_1 G_p - C_T \tag{6.22}$$

where B_1 \$/Kmole and C_T \$/hr are, respectively, the sales value and the total costs. The latter is the sum of the operating costs and capital charges. It can be written as:

$$C_T = B_2 V + B_3 A_h + B_4 F_h + B_5 F C_{af} \tag{6.23}$$

where B_2 \$/(m^3)(hr) and B_3 \$/(m^2)(hr) are, respectively, the costs of the reactor tank and heat exchanger on depreciated basis. B_4 \$/m^3 and B_5 \$/(Kmole) are the costs of the feed and heating fluids respectively. The first two terms in the right hand side of equation (6.23) refer to the capital charges while the last two terms represent the operating costs.

Combination of equations (6.22) and (6.23) yields:

$$P_r = B_1 G_p - (B_2 V + B_3 A_h + B_4 F_h + B_5 F C_{af}) \qquad (6.24)$$

The design data and system constants for the hypothetical case study considered in this chapter are given in table 6.1. The cost factors, B_1, B_2, B_3, B_4 and B_5, are also included in this table. These design data are similar to those used by Gaitonde and Douglas [1969]. Later it will be shown that these parameters result in a highly unstable minimum costs design.

The reactor steady state model, equations (6.1) through (6.7), is composed of seven relationships between ten design variables, F, C_a, V, k, T, Q_h, F_h, T_o, A_h and T_{av}, and other specified quantities. Therefore, any three of the ten design variables can be selected arbitrarily but our aim, in this section, is to find the values which maximize the profit function, equation (6.24), subject to the system equality and inequality constraints. C_a, T and

T_o are here selected as these free variables.

Table 6.1 Design parameters

Design data:	$E_a=2.52875\times10^5$, $(-\Delta H)=2.46707\times10^4$,
	$C_pe=4.19\times10^3$, $C_{ph}e_h=4.19\times10^3$, $k_o=1.4738\times10^{35}$,
	$G_p=2.7$, $T_f=300$, $T_h=373$, $U_c=2.095\times10^4$,
	$C_{af}=10$, $R_g=8.38$
Cost factors:	$B_1=4.4\times10^2$, $B_2=1.0389\times10^2$, $B_3=1.81\times10^3$,
	$B_4=10$, $B_5=1.207$.

No inequality constraints are given as design specifications. However, due to the fact that upper and lower bounds on the adjustable variables are required by the complex optimization algorithm, which is, unless otherwise stated, employed in the solution of all optimization problems in this chapter, the inequalities given below are used. In addition, these upper and lower limits ensure that some nonrealistic designs are not generated. For example, inequality (6.28) below indicates that the temperature of the reacting mixture can not exceed the outlet temperature of the heating fluid.

$$0 < C_a < 10 \tag{6.25}$$

$$301 < T < 372 \tag{6.26}$$

$$301 < T_o < 372 \tag{6.27}$$

$$0 < T/T_o < 1 \tag{6.28}$$

A number of feasible sets of values of the three variables, C_a, T, and T_o, generated using the "FEASBL" subroutine, have been used to start the "complex" optimization algorithm. All the runs have converged to the same solution, namely (C_a=2.2234, T=366.658, T_o=371.668), which yields a global maximum profit of 194.2 \$/hr. When the initial vector (C_a=4.05, T=301.48, T_o=310.55) has been employed, the optimization algorithm required a total number of 167 iterations to find the optimal solution. Figure 6.2 is a plot of the normalised profit versus the iteration number. An iteration number is defined as the calculations required to find a new point which satisfies the constraints and does not repeat in yielding the lowest profit value. The points in the initial complex are also counted as iterations. In figure 6.2, the first fifteen points have not been included due to the very large loss associated with them.

The optimum design variables are given in table 6.2 where the maximum profit design is referred to as design A.

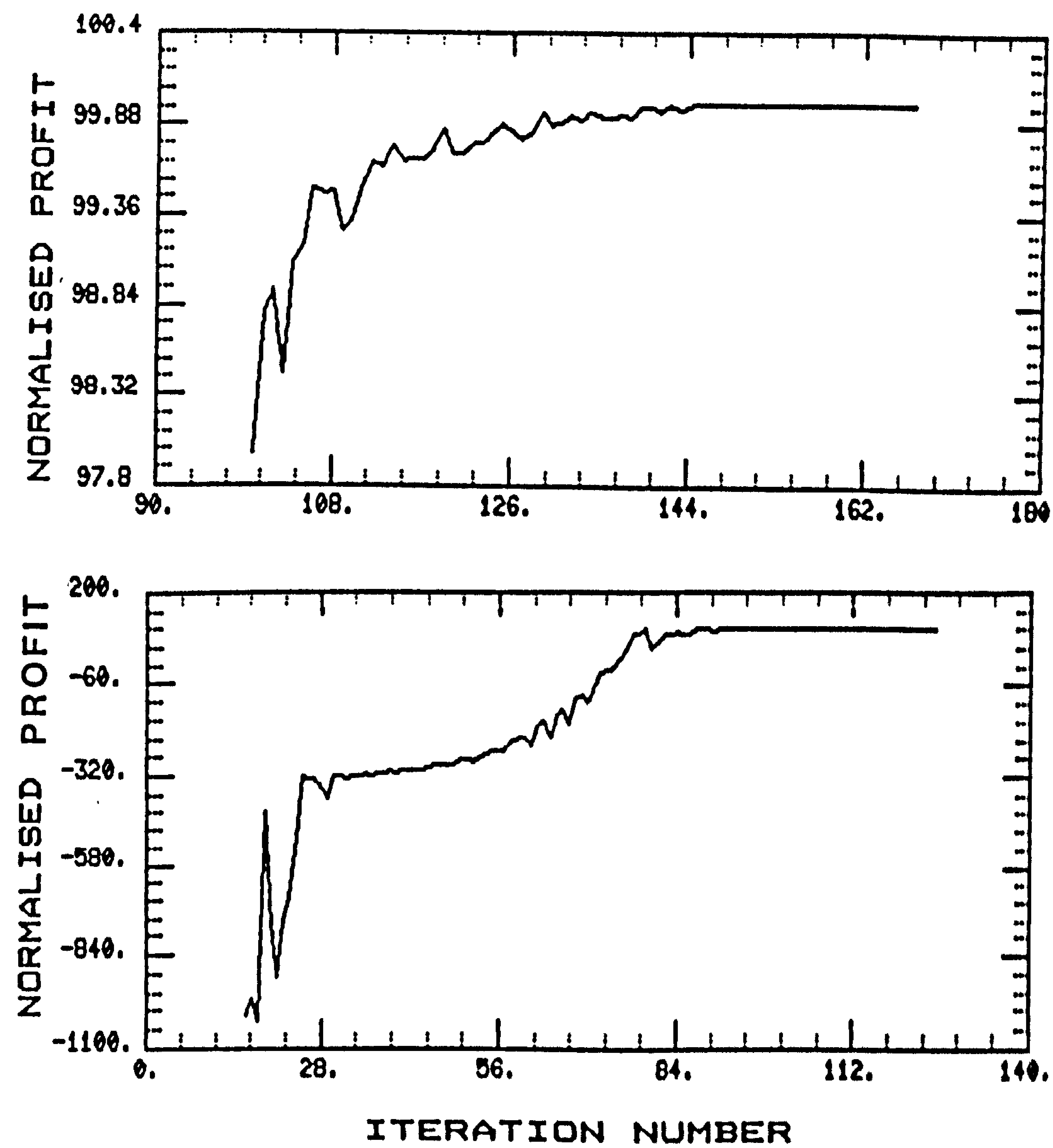


Figure 6.2 Normalised profit, $\bar{P}_r$, versus iteration number

$$\bar{P}_r = (P_r/|194.2|)*100$$

Optimization parameters:

Convergence tolerence = $1.0\text{x}10^{-6}$
Number of points in the "complex" = 6
Reflection factor = 1.3

Table 6.2 Design A

C_a=2.2234,	T=366.658,	T_o=371.668,	A_h=0.25514,
V=4.5575,	F=0.3472,	F_h=5.4349,	Q_h=3.0333x10^4,
k=0.2666,	T_{av}=372.334		

6.5 Stability and open loop behaviour of design A

Using table 6.2 and equation (6.19) the characteristic equation of design A is found to be:

$$D(s) = 0.112s^2 - 0.1666s + 1 \tag{6.29}$$

The roots of equation (6.29) are $0.75 \pm 2.91j$, which indicate that the maximum profit design is unstable.

By setting the time derivatives in equation (6.8) and (6.9) to zero the following steady state relationships are obtained:

$$\frac{F}{V}(C_{af} - C_a) - kC_a = 0 \tag{6.30}$$

$$\frac{F}{V}(T_f - T) + \frac{(-\Delta H)}{C_p e} kC_a$$

$$+ \frac{U_c A_h L F_h}{V C_p e(1+LF_h)}(T_h - T) = 0 \tag{6.31}$$

Equation (6.30) can be solved for C_a to yield:

$$C_a = \frac{F C_{af}}{F+kV} \tag{6.32}$$

By substituting (6.32) into (6.31) and manipulating the resultant relationship we obtain:

$$\left[1 + \frac{U_c A_h L F_h}{F C_p e(1+LF_h)}\right] T - \left[T_f + \frac{U_c A_h L F_h}{F C_p e(1+LF_h)} T_h\right]$$

$$= \frac{(-\Delta H) C_{af}}{C_p e}\left(\frac{kV/F}{1+kV/F}\right) \tag{6.33}$$

Terms on the left hand side of this last equation are related to the heat removed by the convective flow of the processing stream and the heat added through the exchanger (coil). The right hand side of equation (6.33) is related to the heat generated by the chemical reaction. Figure 6.3 is a plot of the two sides of the equation against T_s -- a Van Heerden type diagram.

Since there is only one steady state solution -- a single intersection of the two curves -- which is unstable, the reactor, if disturbed, will exhibit a limit cycle response.

The responses of the reactor nonlinear model to perturbations in the initial conditions are shown in

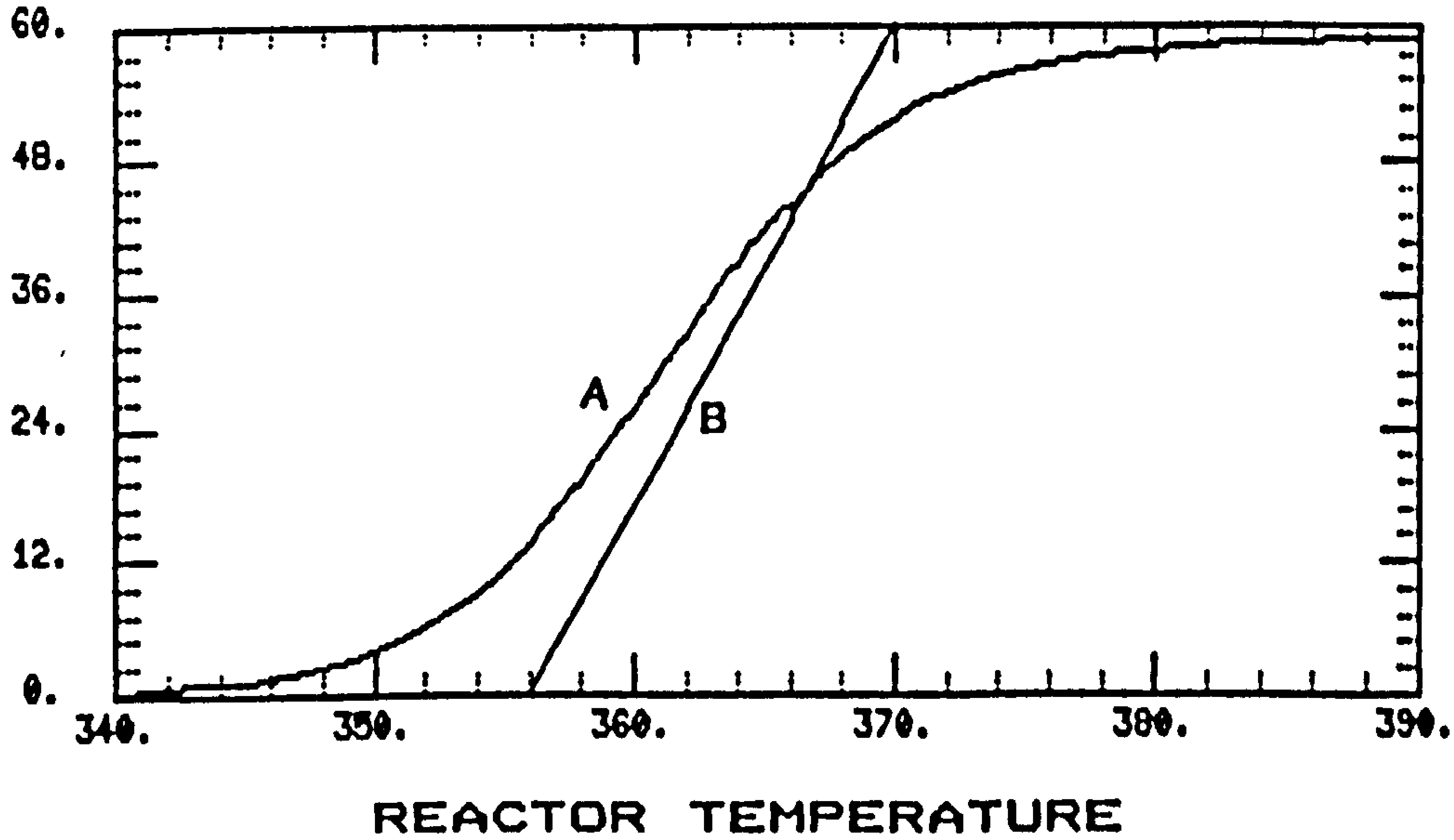


Figure 6.3 Van Heerden diagram

Curve A --- right hand side of equation (6.33)

Curve B --- left hand side of equation (6.33)

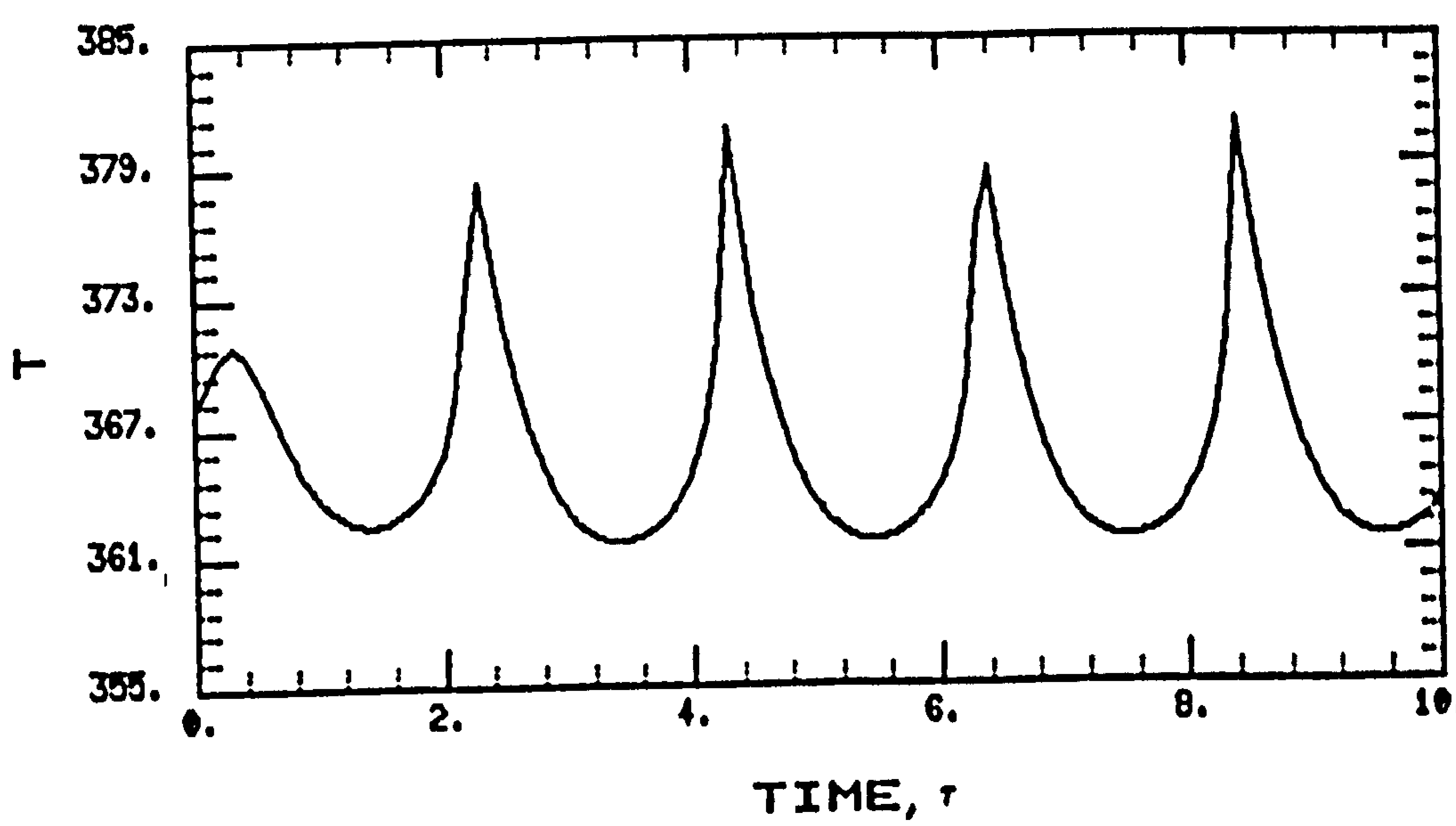


Figure 6.4

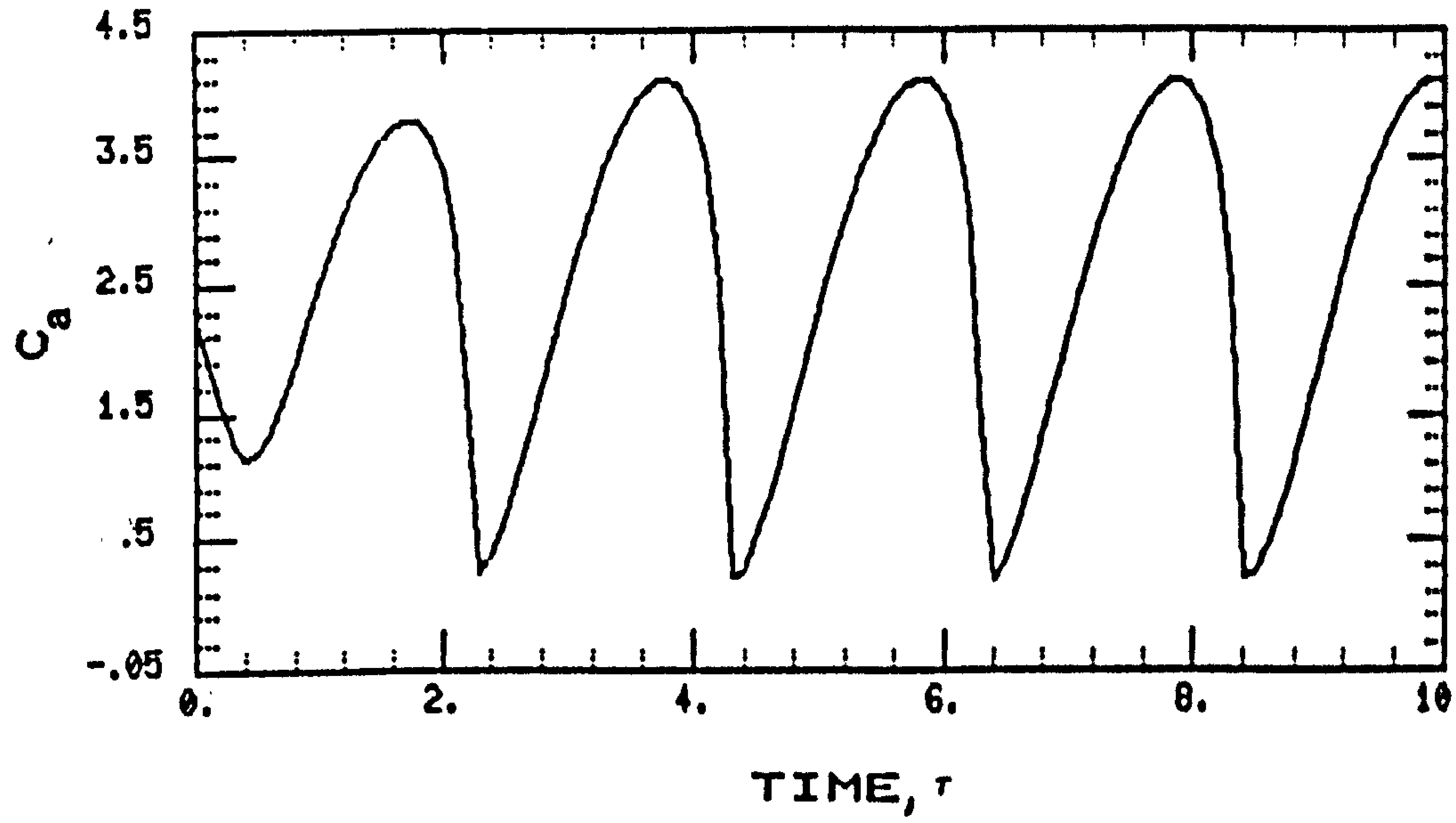


Figure 6.5

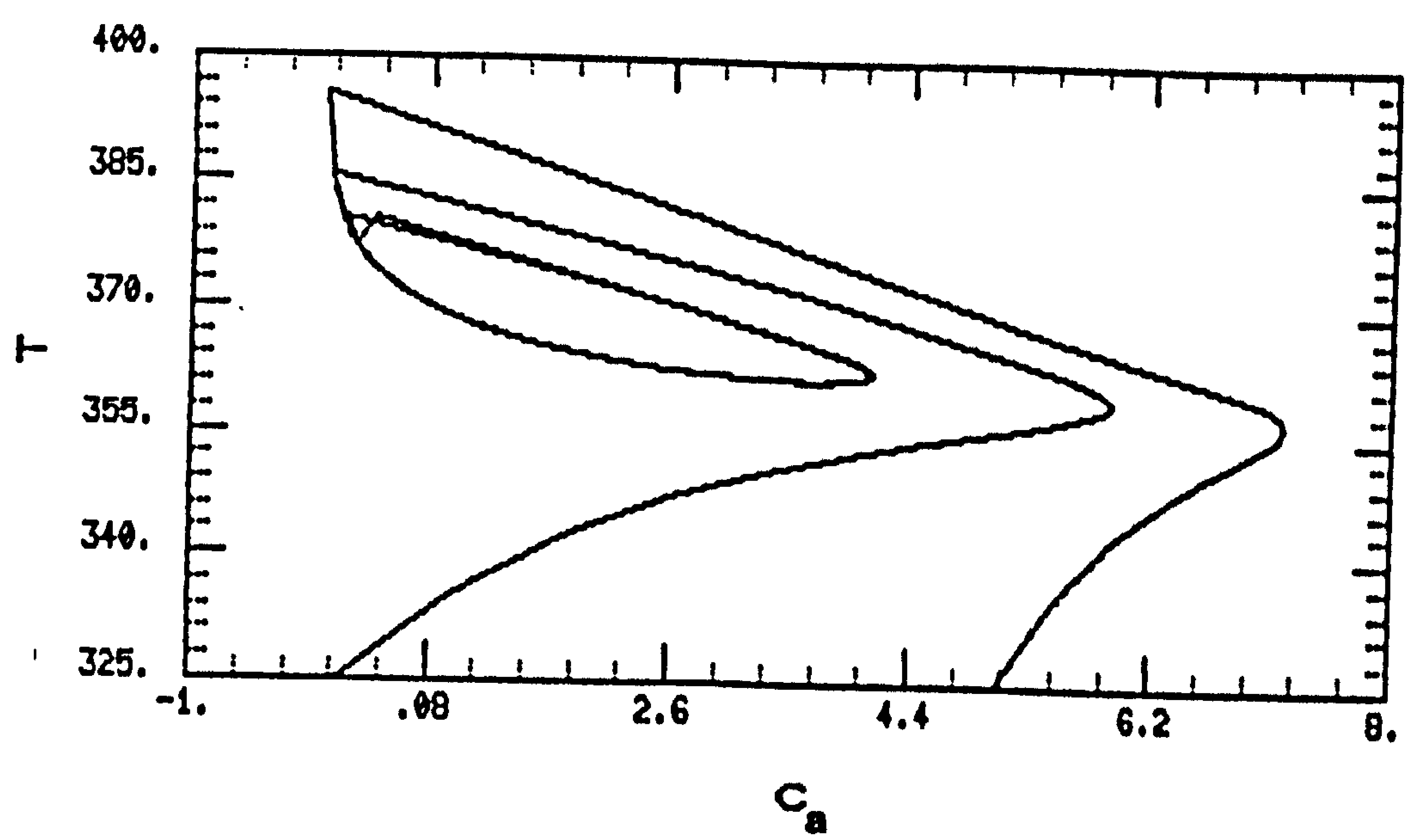


Figure 6.6

figures 6.4 through 6.6. Figures 6.4 and 6.5 are, respectively, the temperature and concentration time responses to a small perturbation in T, whereas figure 6.6 is a phase plane plot of the reactor responses to perturbations in T and C_a. The reactor oscillates between temperatures of 381 ^{o}K and 362 ^{o}K, and concentrations of 0.17 Kmole/m^3 and 4.12 Kmole/m^3. Such a behaviour is here considered unacceptable.

6.6 Integrated design and control of system 1:

6.6.1 System

The flowsheet of the considered controlled plant is as shown in figure 6.7. The reactor temperature is controlled by manipulating the heating liquid flow rate and the major expected disturbances entering the system are in the temperature of the feed stream. The plant controller is Proportional plus Integral (PI).

Using the general dynamic model representing a CSTR, equation (6.15), the considered SISO plant linear model is:

$$X_2(s) = \{g_{22}(s)U_2(s) + g_{24}(s)U_4(s)\}/D(s) \qquad (6.34)$$

This model has been developed on the basis that the heating coil dynamics are negligible. Also equation (6.34) does not include the lags introduced by the valve and the measuring device (thermocouple). To allow for the control difficulties caused by these small lags, a small time delay

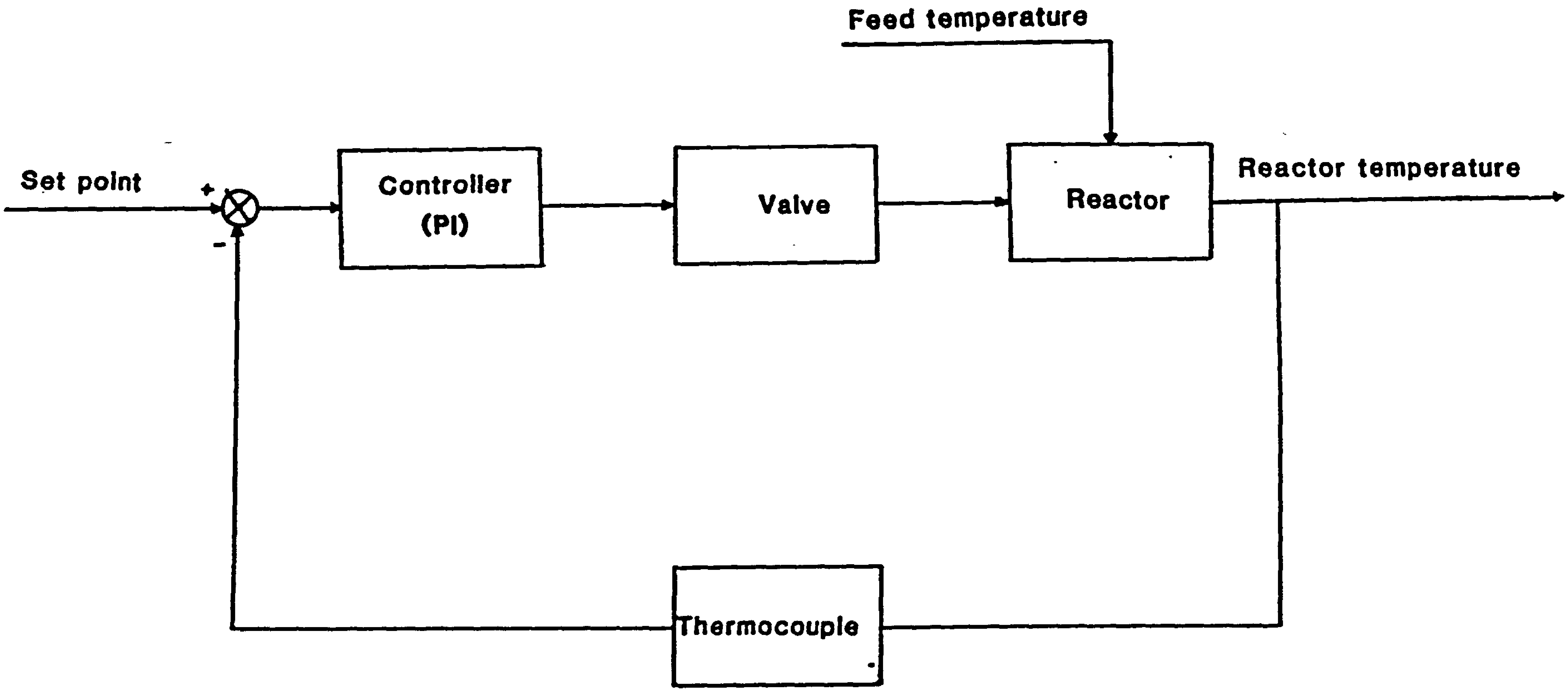


Figure 6.7 Block diagram of system 1

equal to 5% of the reactor natural period, is added to the forward path of the control loop. Experimental work carried out by Huang et al. [1984] have indicated the presence of even higher time delays. Therefore the complete linear model of the plant is:

$$X_2(s) = \{g_{22}(s)\exp(-T_d s)U_2(s) + g_{24}(s)U_4(s)\}/D(s) \quad (6.35)$$

where $T_d=0.05T_p$.

The best values of the controller parameters, the proportional gain and the reset time, are chosen as those values which minimize the overall closed loop performance index ITAE (the Integral of Time Multiplied by the Absolute value of the Error) when the system is subjected to a step change in the feed temperature. ITAE is chosen since, compared with the other commonly used error criteria, it usually results in a less oscillatory optimum response. The pattern search method of Hooke and Jeeves [1961], described in chapter 4, is used to locate the optimum value of the performance index with ISIM employed as the simulation tool for numerically calculating the objective function, ITAE.

In chapter 5 it has been stressed that the use of overall performance indices will not, in most cases, yield the best controller parameters and that the performance of the obtained controller differs from case to case. However, at the plant design stage we are mainly interested in comparing the overall closed loop behaviour of different feasible designs rather than obtaining the best performance of the final design. In addition, the use of overall indices greatly facilitates such a comparison when the plant control system consists of more than one loop. For these reasons, the use of ITAE and similar criteria for ranking the closed loop behaviour of different plant designs is justified.

6.6.2 Design criteria

The design criteria used for ordering the feasible set of reactor designs together with their values at the maximum profit design are given in table 6.3. The rate of profit, P_r, is a measure of the steady state economic performance of the plant. The other attributes are related to the reactor open loop and closed loop dynamic behaviour. The open loop damping, ζ ,is used to indicate the uncontrolled reactor degree of stability and the speed at which a runaway might occur. $\bar{T}$ gives the minimum and maximum values of temperature between which an open loop reactor design, represented by its nonlinear model, will limit cycle. Their concentration counterpart values are given by $\bar{C}$. The importance of these two pairs, $\bar{T}$ and $\bar{C}$, is highly dependent on the frequency at which the controller fails, characteristics like the reactants and catalyst sensitivity to temperature, and the nature of downstream plant units. The minimum ITAE (MITAE or ME) is used as a measure of the overall quality of control. Its value is dependent on the time scale used for its evaluation. Therefore, a common time scale has to be used if this criterion is to be employed for comparing, without distortion of the conclusions drawn, the closed loop dynamic behaviour of different designs. All the ME values given in this chapter are based on real time which are the result of multiplying their corresponding values obtained from simulation of system 1 by the square of the reactor residence time, V/F. Note that the plant in system 1 is represented by equation (6.35) which is based on dimensionless time.

Since the design which yields maximum profit is highly unstable, obtaining a reactor which has a much improved open loop dynamic behaviour would be a major concern of the designer. The damping of the uncontrolled reactor is here considered as a primary criterion.

Table 6.3 Design criteria and their values at design A

P_r=194.2, ζ=-0.249, ME=$4.125\mathrm{x}10^{-4}$, $\tilde{T}$=(362,381), $\bar{C}_a$=(0.17,4.12).

6.6.3 Maximum damping

The damping maximization problem has the same formulation as the profit maximization problem except that, in this case, the damping of the open loop system, ζ , is used as the objective function. Initial attempts, however, have shown that in order to obtain a realistic solution to such a problem, additional constraints on the design variables are needed. Using the constraints given below to further reduce the set of feasible designs, the maximum open loop damping of the reactor is found to be 0.404. The characteristics of the design yielding this highest value are given in table 6.4.

$$0 < A_h \leqslant 0.44 \tag{6.36}$$

$$0 < V \leqslant 5.2 \tag{6.37}$$

Table 6.4 Characteristics of design B

Design variables:	$C_a=0.8703$, $T=370.279$, $T_o=372.0$,
	$A_h=0.44010$, $V=5.2003$, $F=0.2957$,
	$F_h=4.9052$, $Q_h=2.0553\times10^4$,
	$k=0.59663$, $T_{av}=372.5$
Design criteria:	$P_r=-201.6$, $\zeta=0.404$, $ME=2.64\times10^{-5}$,
	$\bar{T}=$ ——, $\bar{C}=$ ——

As indicated in the proposed design algorithm, another approach for obtaining a second extreme nondominated solution would have been to solve the original profit maximization problem with an additional constraint on the open loop reactor damping instead of maximizing the latter criterion.

A value of the reactor damping equal to 0.404 indicates that design B, if disturbed, will exhibit an underdamped stable response. The responses of the nonlinear model of design B to perturbations in the initial conditions are shown in figures 6.8 through 6.10. Figure 6.8 and 6.9 are, respectively, the time responses of the temperature and concentration of the processing stream leaving the reactor to a small perturbation in T, whereas figure 6.10 is a phase plane plot of the reactor responses to perturbations in T and C_a.

An examination of tables 6.3 and 6.4 shows that, compared to design A, design B exhibits 262.3% (from ζ=-0.249 to ζ=0.404) increase in the open loop damping, 203.8% (from a profit of 194.2 to a loss of -201.6) reduction in the steady state profit and 93.6% (from ME=4.125×10^{-4} to ME=2.64×10^{-5}) reduction in the overall closed loop performance index. The large improvement in the quality of control exhibited by design B indicates that the open loop reactor damping is not only a measure of the plant degree of stability but also a measure of its degree of controllability.

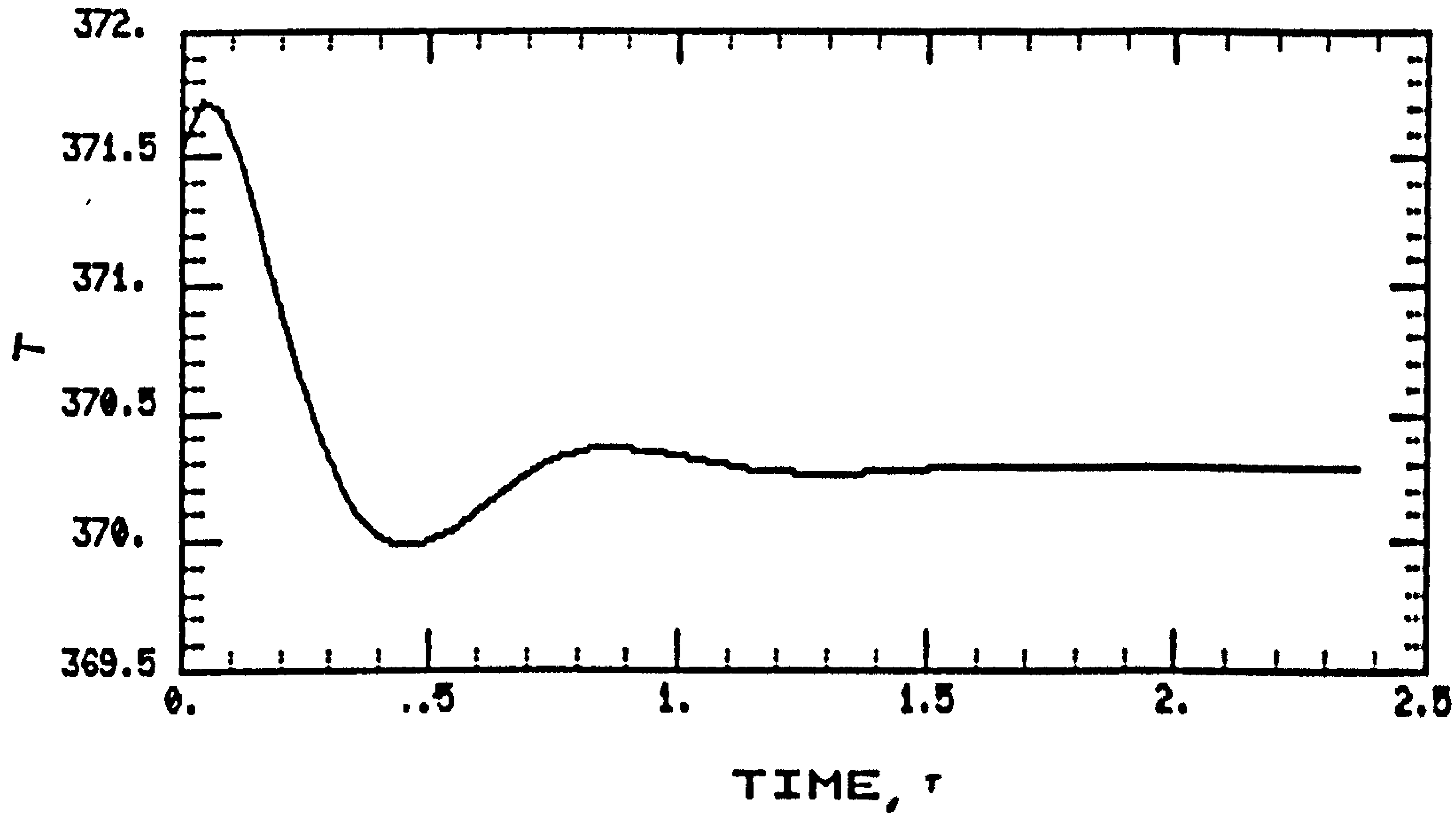


Figure 6.8

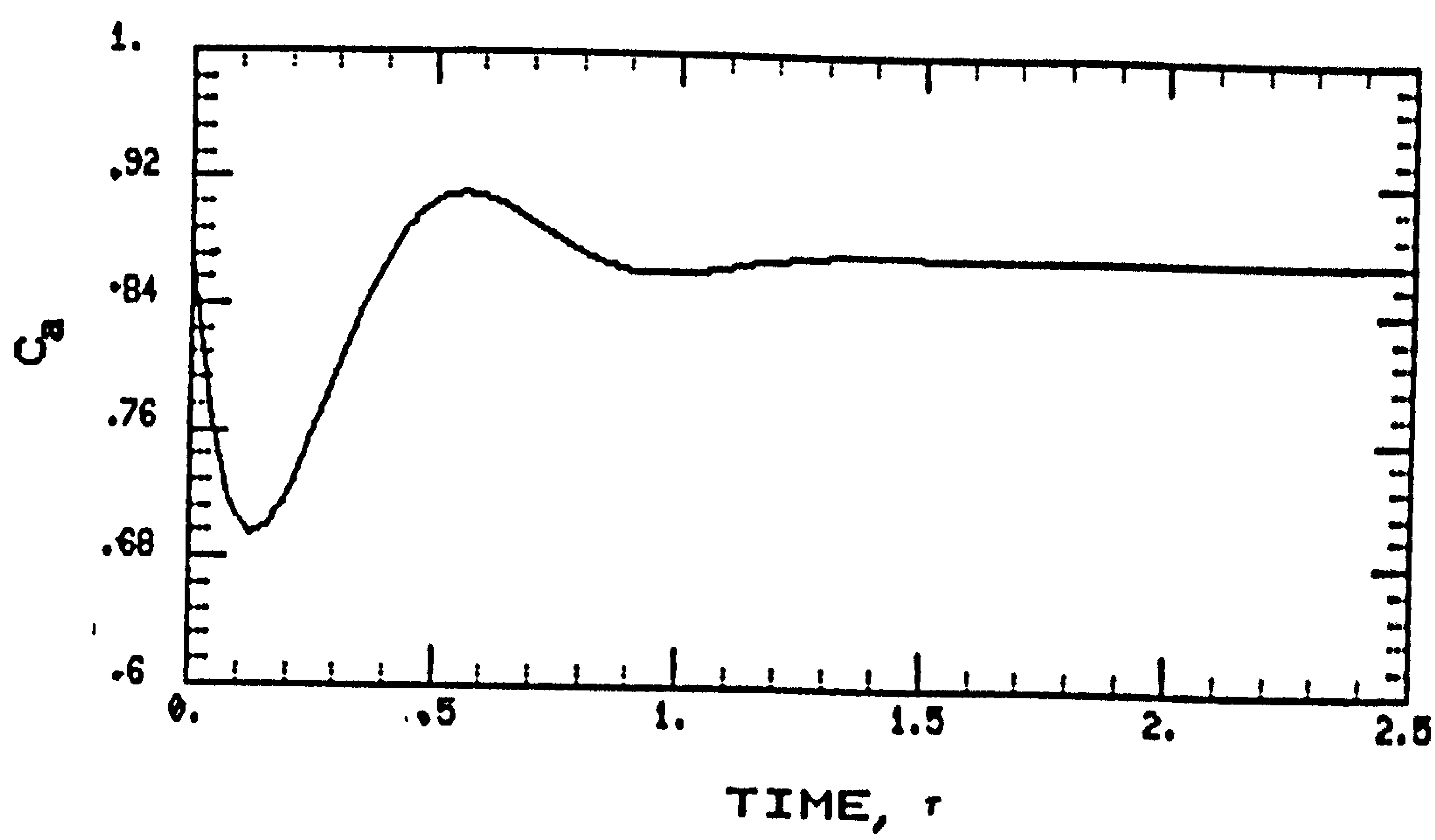


Figure 6.9

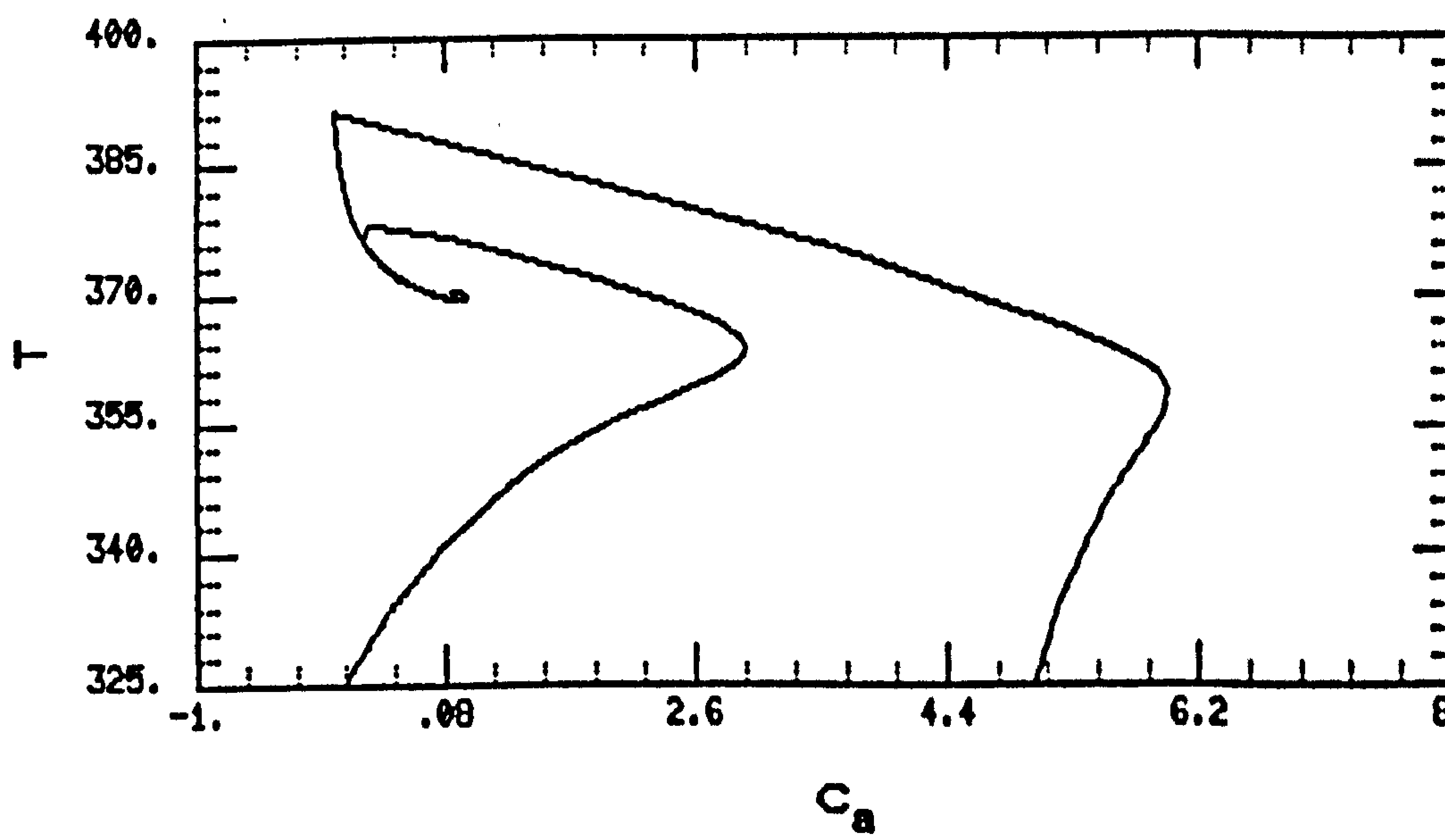


Figure 6.10

The $\bar{T}$ and $\bar{C}$ criteria are measures of the size of the limit cycle response of an open loop design to external and internal upsets and hence they are not expected to be in conflict with ζ. Therefore, in what follows the steady state profit and the open loop reactor damping are considered as primary criteria, and the other dynamic attributes, $\bar{T}$, $\bar{C}$ and ME, are considered as secondary criteria.

6.6.4 Nondominated set

Using the values of the steady state profit and the open loop reactor damping obtained through the maximization of each of these two criteria, the nondominated set of solutions given in table 6.5 and plotted in figure 6.11 has been generated as outlined in the proposed design algorithm, see section 3.2, with the steady state profit as the objective function and the damping as the additional inequality constraint to the set of constraints defining the feasible region. The secondary criteria are plotted in figure 6.12 through 6.14. Figures 6.15 and 6.16 give the reactor and the heat exchanger (coil) sizes as they vary with the nondominated set. The overhead bar is used to indicate that the criterion or design variable is normalised by dividing it by its absolute value at the maximum profit design and multiplying the result by 100, eg. $\bar{\zeta}=(\zeta/|-0.249|)*100$. It is interesting to note that initially, as we move away from design A, a tank underdesign rather than overdesign is required. To obtain a stable solution, a 1% reduction in the reactor volume and only 8% increase in the heating coil are needed.

Table 6.5 Nondominated set

solution (C_a, T, T_o)	$\overline{P}_r$	$\overline{r}$
S1 (2.2234,366.658,371.668)	100.0	-100.0
S2 (2.1150,366.952,371.721)	99.2	-80.3
S3 (1.8800,367.570,371.851)	93.5	-40.2
S4 (1.6245,368.094,371.969)	80.2	0.0
S5 (1.3706,368.553,372.00)	60.2	40.2
S6 (1.1588,368.989,372.00)	30.0	80.3
S7 (1.0113,369.596,372.00)	-16.4	120.5
S8 (0.8703,370.279,372.00)	-103.8	162.3

Now that the noninferior set and the secondary criteria charts are available, the decision's maker (designer) task

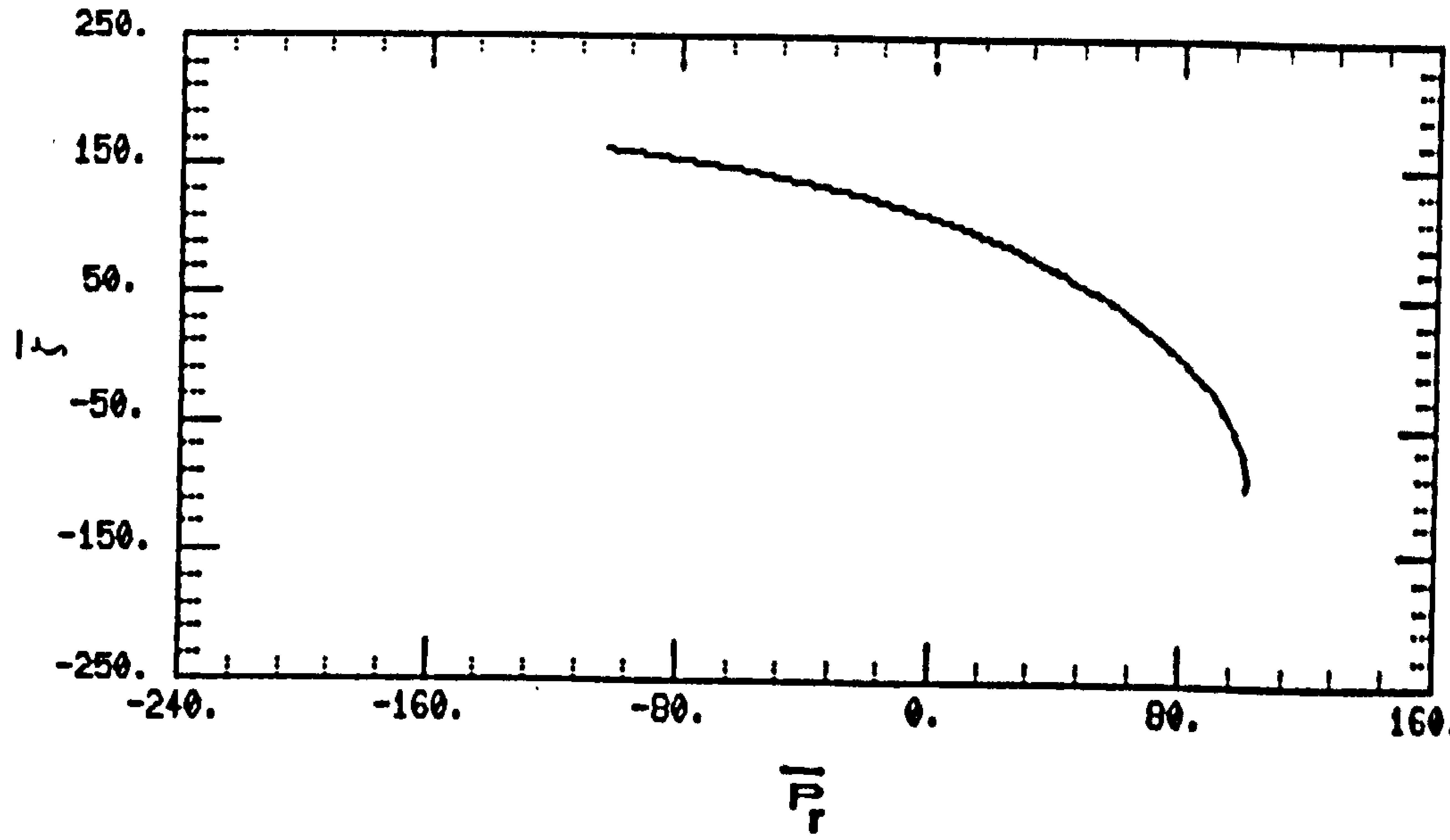


Figure 6.11 Nondominated set

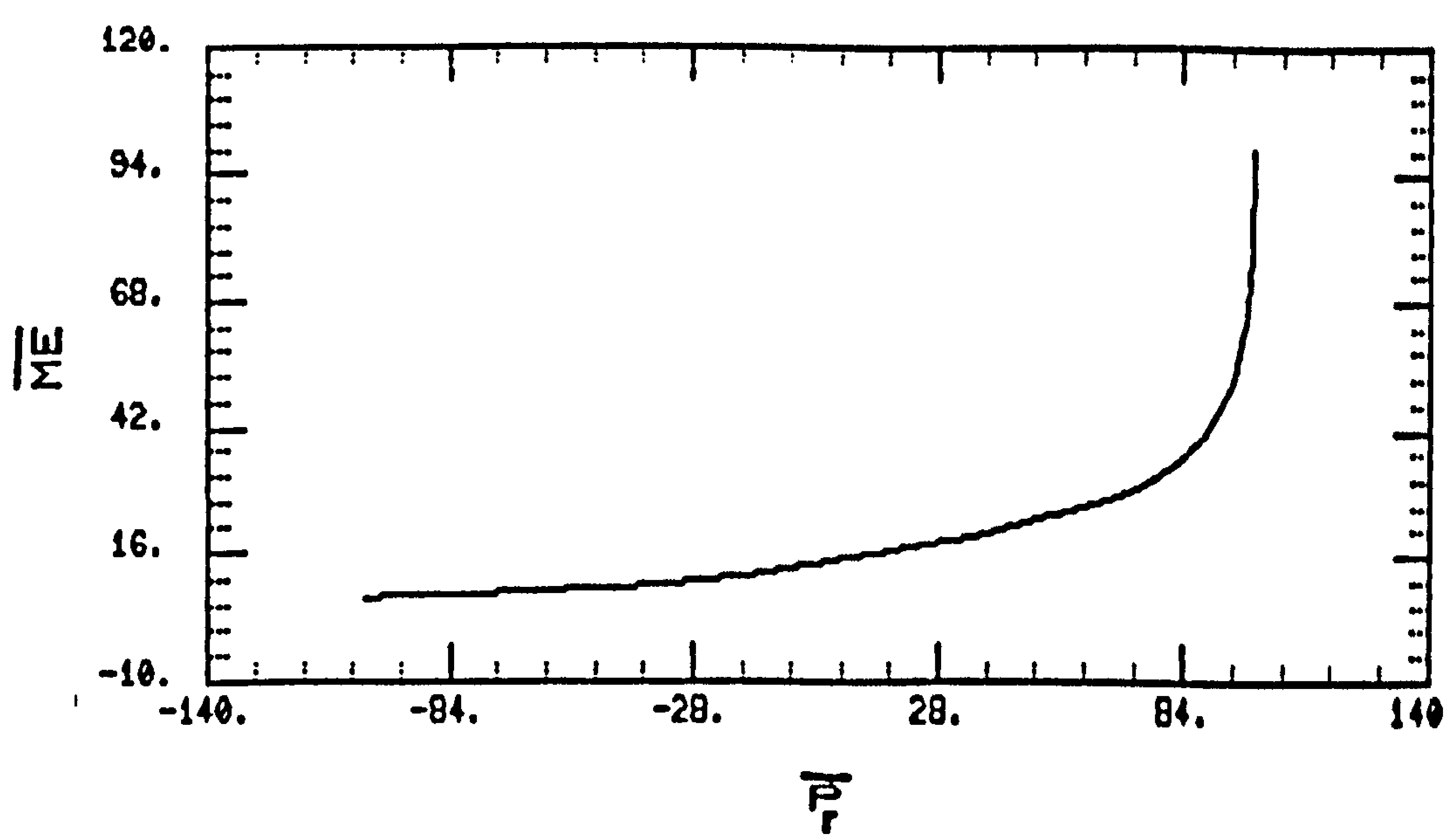


Figure 6.12 Variation of the overall closed loop performance with the nondominated set

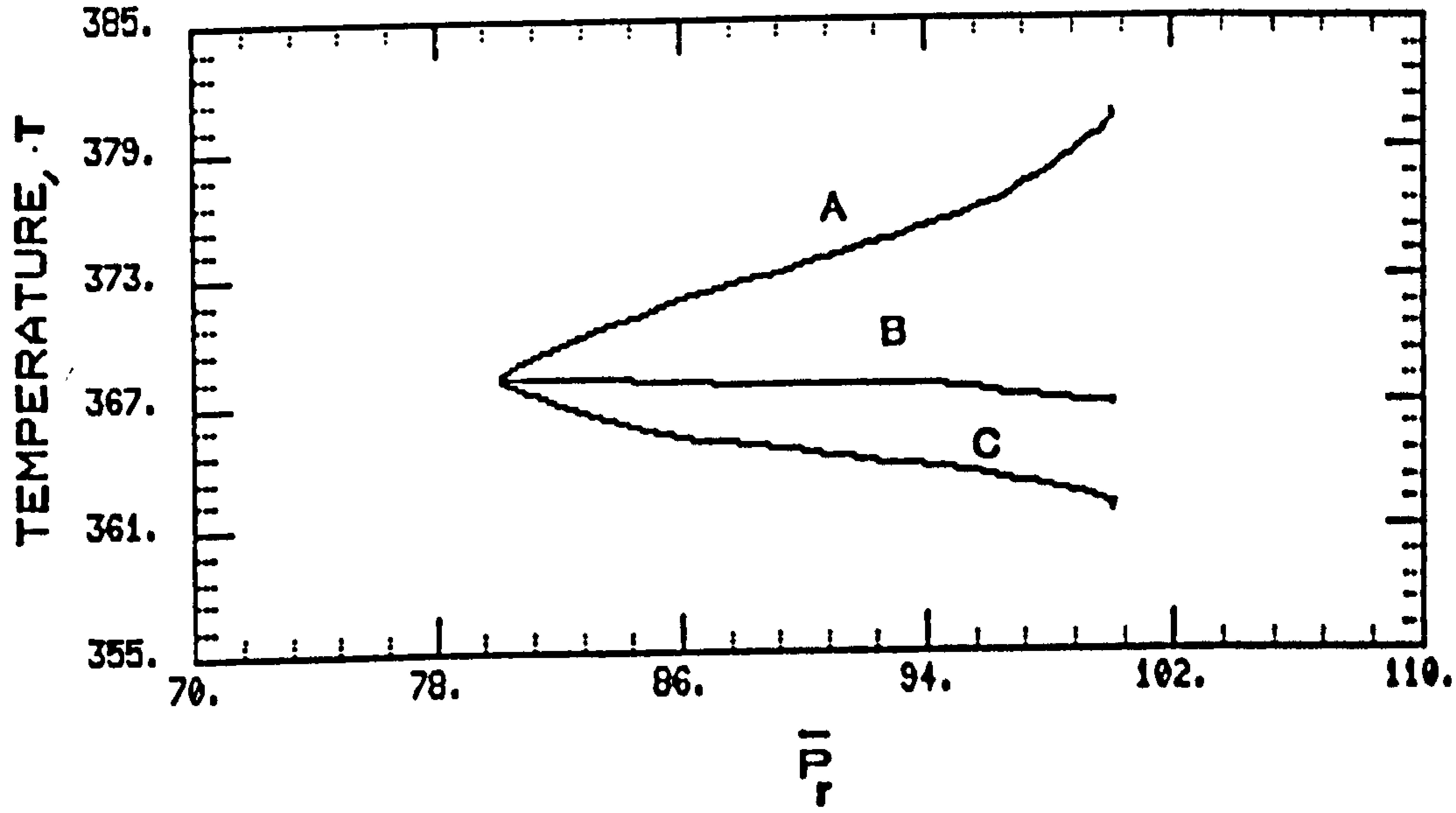


Figure 6.13 Variation of $\tilde{T}$ with the nondominated set

Curve A --- maximum temperature/concentration

Curve B --- operating temp./concn.

Curve C --- minimum temp./concn.

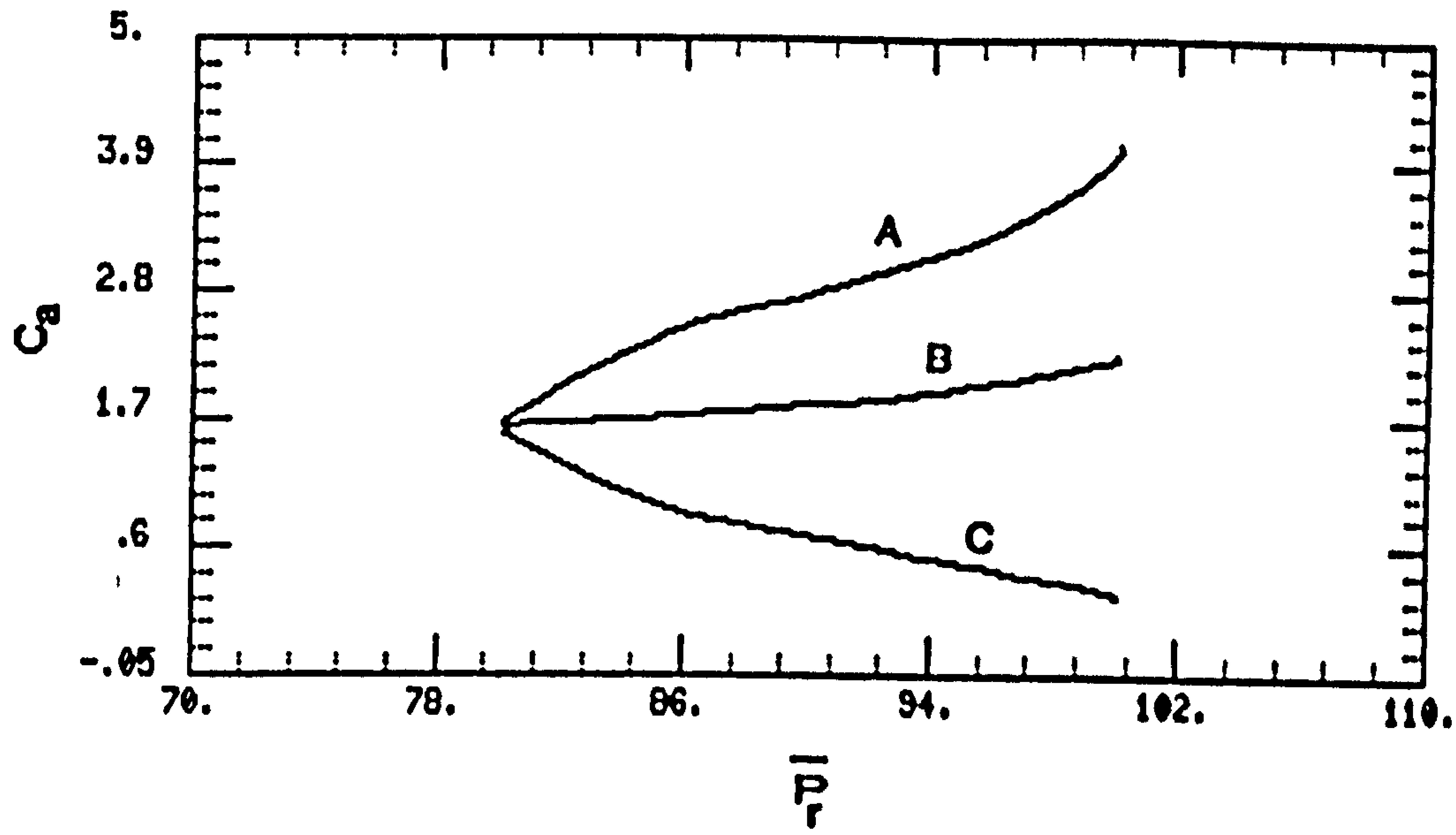


Figure 6.14 Variation of $\tilde{C}_a$ with the nondominated set

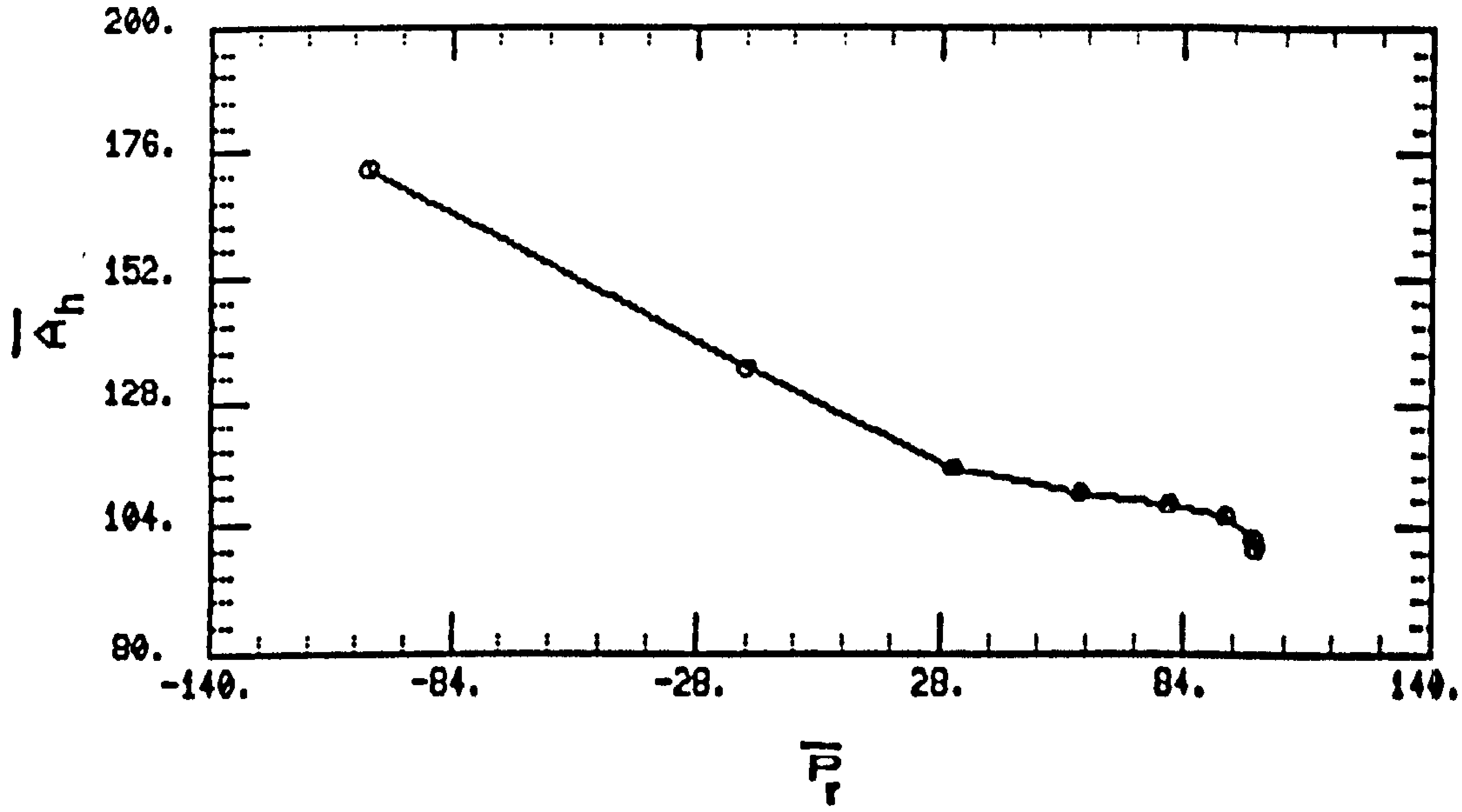


Figure 6.15

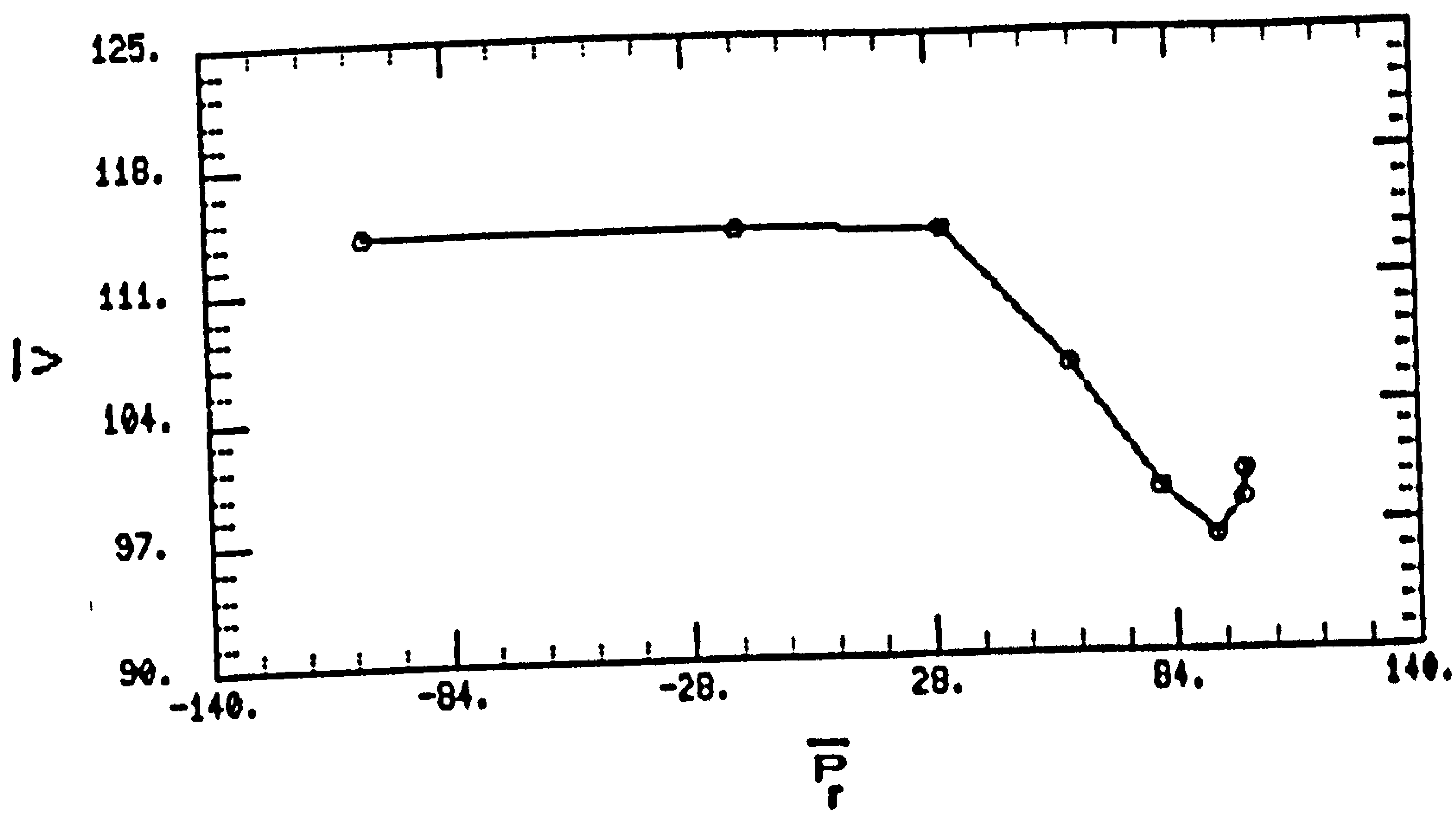


Figure 6.16

is to choose the best design. The process of decision making, here, is equivalent to converting the dynamic criteria into monetary terms (pounds or dollars) in a fuzzy manner. To do so the designer uses additional quantitative and qualitative criteria which are measures of safety, technological or even political attributes. Catalyst decay, the sensitivity of the reactants to temperature and enviromental regulations are few examples. The nature of interaction between the reactor and other units of the overall plant is another attribute from which the designer extracts some information about the importance of good open loop and closed loop dynamic behaviour of the reactor.

Although it has been stressed in the above discussion that the choice of the final design rests with the decision maker as other quantitative and subjective criteria need to be accounted for, and that any nondominated solution may be chosen as the best design, a preliminary analysis may reduce the number of candidate designs. The following mathematical model has been found to represent the nondominated set of solutions with a very good accuracy:

$$\bar{\zeta}' = \begin{cases} -45.67\bar{P}_r + 4467 & 99.7 < \bar{P}_r \\ -9.5\bar{P}_r + 860.85 & 96.5 < \bar{P}_r \leqslant 99.7 \\ -0.105\times10^{-5}(\bar{P}_r)^4 + 0.42\times10^{-4}(\bar{P}_r)^3 - & \\ 0.23\times10^{-2}(\bar{P}_r)^2 - 0.91\bar{P}_r + 108.6 & \bar{P}_r \leqslant 96.5 \end{cases} \qquad (6.38)$$

The gradient of which is given by:

$$d\bar{\zeta}/d\bar{P}_r = \begin{cases} -45.67 & 99.7 < \bar{P}_r \\ -9.5 & 96.5<\bar{P}_r\leqslant 99.7 \\ -0.42\times10^{-5}(\bar{P}_r)^3 + 1.26\times10^{-4}(\bar{P}_r)^2 & \\ 0.46\times10^{-2}(\bar{P}_r) - 0.91 & \bar{P}_r \leqslant 96.5 \end{cases} \qquad (6.39)$$

Consider designs C and D given below in tables 6.6 and 6.7, which are at the intersections of the three nondominated set regions defined as:

region I: $96.5<\bar{P}_r$

region II: $60<\bar{P}_r\leqslant 96.5$

region III: $\bar{P}_r\leqslant 60$

In design C significant improvements in the process dynamics are obtained at the expense of a marginal loss in the predicted steady state profit. A mere 3.5% reduction in the maximum profit results in 44.1% increase in the uncontrolled reactor damping and 37% improvement in the overall closed loop performance index, ME. As indicated by equation (6.39), the gradient, in region I over 9.5% increase in the damping is traded off for every 1% reduction in the profit. In most cases such a tradeoff is accepted and this region is excluded from further consideration. Design D is open loop stable and it represents a large reduction in the steady state profit. Furthermore, in region III only 1.64%, or less, increase in the damping can be obtained for every 1% reduction in the profit. This tradeoff is rarely accepted particularly when the steady state profit is considerably lower than its maximum possible value and the plant dynamics are acceptable. Therefore region III may also be eliminated from further consideration. This means that the candidate solutions for the best design are those belonging to region II. Assume that design E (solution S3 in table 6.5) is chosen by the designer as the best solution. The characteristics of this design are given in table 6.8.

Table 6.6 Characteristics of design C

Design variables:	$C_a=1.9956$, $T=367.321$, $T_o=371.795$,
	$A_h=0.26829$, $V=4.3739$, $F=0.3373$,
	$F_h=5.6512$, $Q_h=2.8533\times10^4$,
	$k=0.3096$, $T_{av}=372.398$
Design criteria:	$\overline{P}_r=96.5$, $\overline{\zeta}=-55.9$, $\overline{ME}=63.0$,
	$\overline{T}=(363.3,376.7)$, $\overline{C}_a=(0.37,3.37)$

Table 6.7 Characteristics of design D

Design variables:	C_a=1.3706, T=368.553, T_o=372.0,
	A_h=0.28131, V=4.8369, F=0.3129,
	F_h=5.5733, Q_h=2.3352x10^4,
	k=0.4071, T_{av}=372.40
Design criteria:	$\overline{P}_r$=60.0, $\overline{\Gamma}$=40.3, $\overline{ME}$=26.2, $\bar{T}$= ——,
	$\bar{C}_a$= ——

Table 6.8 Characteristics of design E

Design variables:	C_a=1.8800, T=367.570, T_o=371.851,
	A_h=0.27038, V=4.39381, F=0.3325,
	F_h=5.7278, Q_h=2.7575x10^4,
	k=0.3270, T_{av}=372.426
Design criteria:	$\overline{P}_r$=93.5, $\overline{\Gamma}$=-40.2, $\overline{ME}$=50.0,
	$\bar{T}$=(364.0,375.0), $\bar{C}_a$=(0.52,3.04)

Compared to design A (the maximum profit design) design E represents a large improvement in the open loop and closed loop dynamic performance (59.8% increase in the open loop damping and 50% reduction in the measure of the quality of control, ME) at the expense of a relatively small (6.5%) reduction in the steady state profit. The closed loop responses of these two designs to a step change of 0.02 (1.2^{O}K) in the feed temperature, $u_4(t)$, are given in figure 6.17. The superiority of the quality of control obtained from design E is quite apparent in this figure.

6.7 Integrated design and control of system 2

6.7.1 System:

In this section, the design of a system which is composed of a CSTR and its multivariable controller is undertaken. System 2 is based on the following assumptions

(a) It is desired to control both the temperature and concentration of the reactor by manipulating the feed and heating fluid flow rates.

(b) The dynamics of the control valves and measuring devices are negligible.

(c) Changes in all plant forcing inputs are negligible, i.e $u_i(t)=0 \quad i=3,4,5$.

Using the general linear model developed in section 6.3, the plant (reactor and control instrumentation)

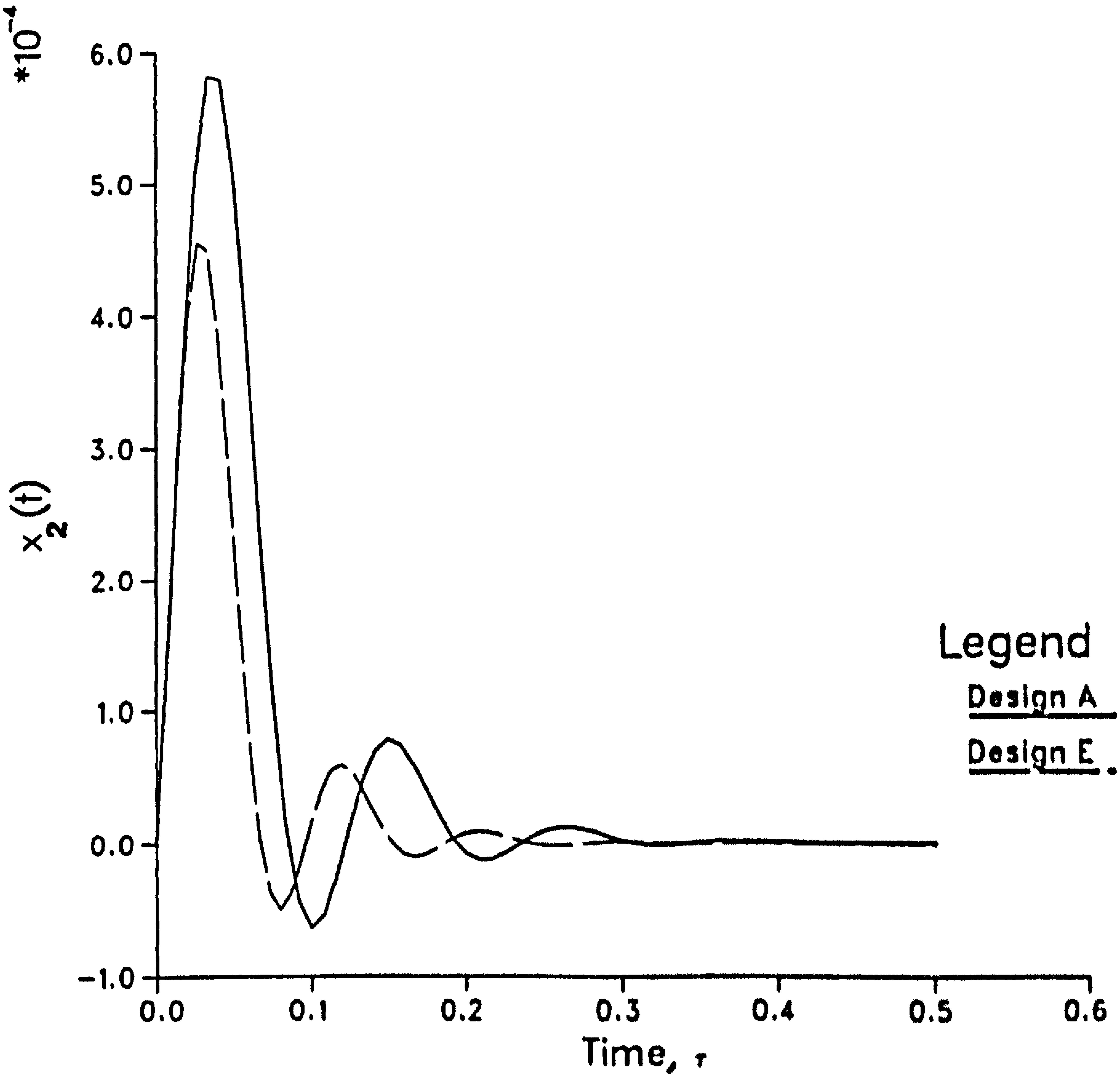

*10⁻⁴
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
$x_2(t)$
0.0
0.1
0.2
0.3
0.4
0.5
0.6
Time, τ
Legend
Design A
Design E

Figure 6.17

dynamics can then be represented by:

$$\dot{x}(t) = Ax(t) + Bu(t) \tag{6.40}$$

where,

$B = [b_{ij}]$ i=1,2; j=1,2

$u^T = [u_i(t)]$ i=1,2

The definition of system 2 is completed by assuming that the plant controller is designed using the well known Linear Quadratic Problem (LQP) formulation.

6.7.2 Controller design

The LQP is a problem for which there exists a closed-form analytical solution for the computation of the optimal state feedback controller and the minimum value of the objective function. This solution can be found in most textbooks on optimal control (e.g Kwakernaak and Sivan [1972], and Jacobson et al. [1980]). What follows in this subsection is based on a plant represented by equation (6.40), however the obtained results apply to all stabilizable time invariant systems.

The LQ Problem is defined as the minimization of the following objective function:

$$J = \int_{0}^{\infty} \{ u^T(t)Ru(t) + x^T(t)Qx(t) \} d\tau \qquad (6.41)$$

Subject to:

$$\dot{x}(t) = Ax(t) + Bu(t) \qquad (6.42)$$

$$x(0) = x_o \qquad (6.43)$$

where Q and R are (2x2) weighting matrices. R must be positive definite and Q may be positive semidefinite. Both matrices are symmetric.

In the above LQP formulation it is assumed that enough time ($t \rightarrow \infty$) is allowed for the system to settle after one or both state variables are perturbed at t=0. The optimal state feedback controller is unique and is given as:

$$u(t) = -Kx(t) \qquad (6.44)$$

where,

$$K = R^{-1}B^TP \qquad (6.45)$$

P is a symmetric and positive definite matrix satisfying the steady state Riccati equation:

$$A^TP + PA - PBR^{-1}B^TP + Q = 0 \qquad (6.46)$$

The minimum value of the objective function, MJ, is given by:

$$MJ = x_o^T P x_o \tag{6.47}$$

The above results can be arrived at through a number of approaches. An easy to follow method is given by Jacobson et al. [1980].

The determination of the optimal controller parameters and the minimum value of the objective function relies on the solution of the matrix Riccati equation. The simple approach used in this study for solving equation (6.46) is outlined in appendix 6A.

The objective function is defined as the integral of a weighted function of noncommensurable and conflicting criteria, namely the state and input variables deviations. The optimal controller and the minimum value of the objective function, and hence the quality of control obtained from a given plant design, are dependent on the weighting factors (the values of the elements of Q and R matrices). A major drawback of the LQ Problem is that no procedure is available for determining the best values of these factors.

To avoid unnecessary complexity, Q and R are here chosen to be diagonal matrices. The elements of these weighting matrices reflect the relative importance attached to the state and input variables. In this study, for comparison reasons, two approaches are used for the determination of the elements of Q and R. In both cases, the cost factor associated with deviations in $x_1(t)$ is assumed to be equal to one, i.e $q_{11}=1$, and the state variables are weighted more heavily than the manipulated variables since the main aim of control is to keep the controlled variables at their respective steady states. In the first approach, 1% change in the reactor concentration, 1% change in the reactor temperature, 10% change in the feed flow rate and 10% change in the heating fluid flow rate are all assumed to contribute equally to the objective function. When the weighting factors calculated on this basis are used for the determination of the best controller, the obtained minimum value of the objective function is referred to as MJA. In the second approach, the elements of Q and R are determined as follows: First, the weighting factors, q_{11}, q_{22}, r_{11} and r_{22}, which represent equal contribution to the objective by a 1% change in each of the manipulated and controlled variables are calculated. Then r_{11} is divided by 10 and r_{22} is divided by 1000. When the resulting factors are used in solving the LQ Problem, the obtained minimum value of the performance index is referred to as MJB.

If different values of the objective function, J, are to be compared they should be calculated using a common time scale. The plant model, equation (6.40), is based on normalised time, τ , and therefore the obtained values of MJA or MJB are also based on τ which is equal to real time, t, divided by the reactor residence time, V/F. The residence time, and hence the time scale, varies from a plant design to another. Therefore a correct comparison of the quality of control, as measured by MJA or MJB, obtained from different systems can be performed only if the calculated values of MJA or MJB are converted to their real time values -- or any other common time scale -- through multiplying them by the residence time of the plant in question. All MJA and MJB values given in this section are those based on real time.

6.7.3 Design criteria and system design

As in system 1 it is here assumed that the damping of the open loop plant, and the two pairs of temperature and concentration, $\bar{T}$ and $\bar{C}$ respectively, measuring the size of the limit cycle exhibited by an unstable design are used as measures of the optimality of the open loop dynamic behaviour. The minimum value of the LQ Problem objective function, MJA or MJB, is used as the overall closed loop performance index and the steady state profit, P_r, is employed to measure the economic performance of the plant.

Assuming that a similar analysis to that carried out in the design of system 1 has led to the choice of the steady state profit and the open loop plant damping as primary criteria and the other dynamic attributes as secondary criteria, the nondominated set is as given in table 6.5 and plotted in figure 6.11, and the secondary criteria are given by figures 6.13, 6.14 and 6.18 or 6.19 depending on whether approach 1 or approach 2 is used by the designer for the determination of the weighting matrices Q and R. At the maximum profit design, MJA and MJB have values of 2.21×10^{-4} and 2.55×10^{-5} respectively. It is interesting to note that although the weighting factors used for the calculation of MJA and MJB are quite different, these two indices give a similar ranking of the nondominated set. If it is again assumed that solution S3 (design E) given in table 6.5 is chosen as the best design, the quality of control as measured by either MJA or MJB represents a large improvement (reductions of 28.8% and 29.8% in MJA and MJB respectively) over that obtained from the maximum profit design.

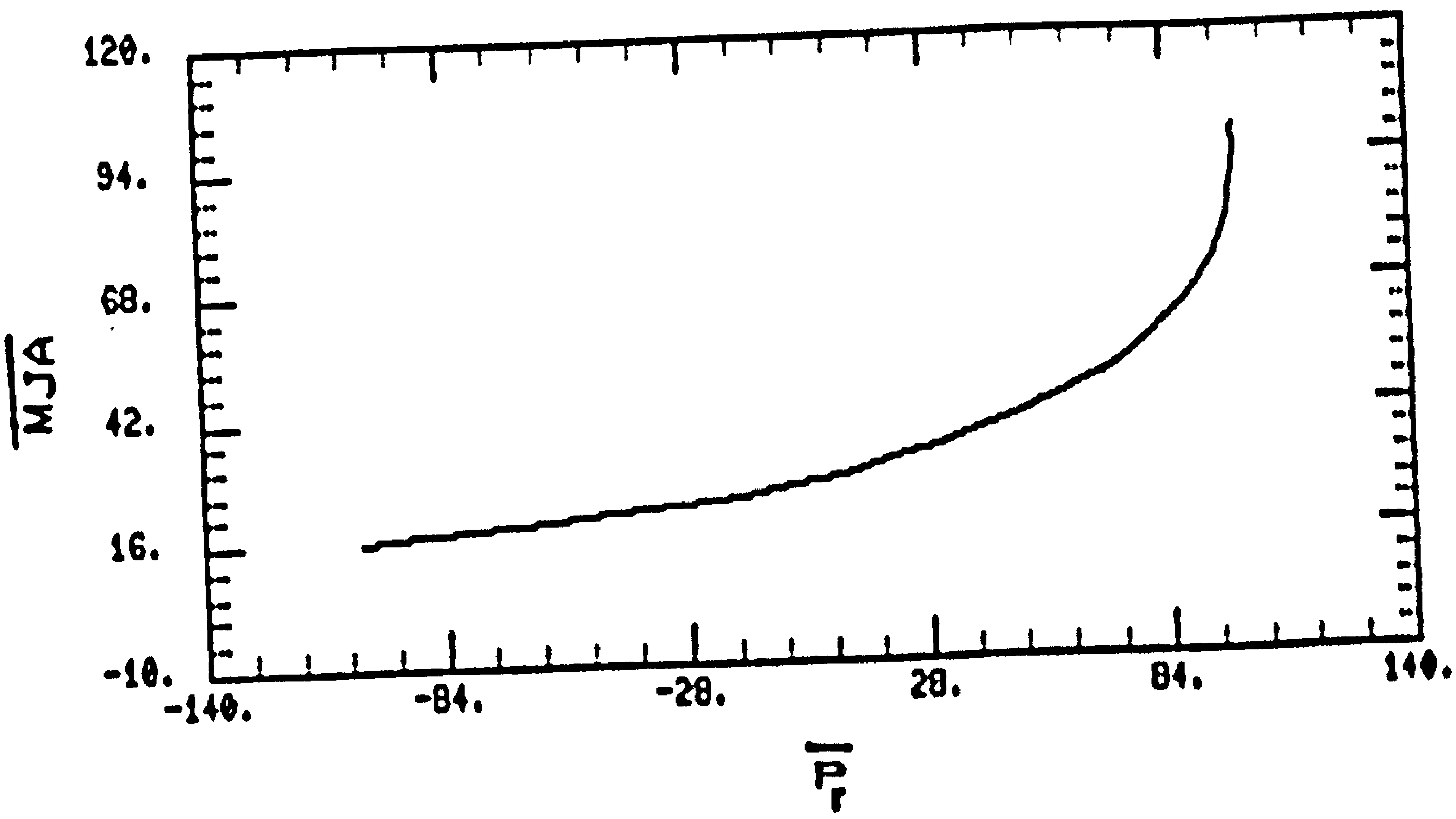


Figure 6.18

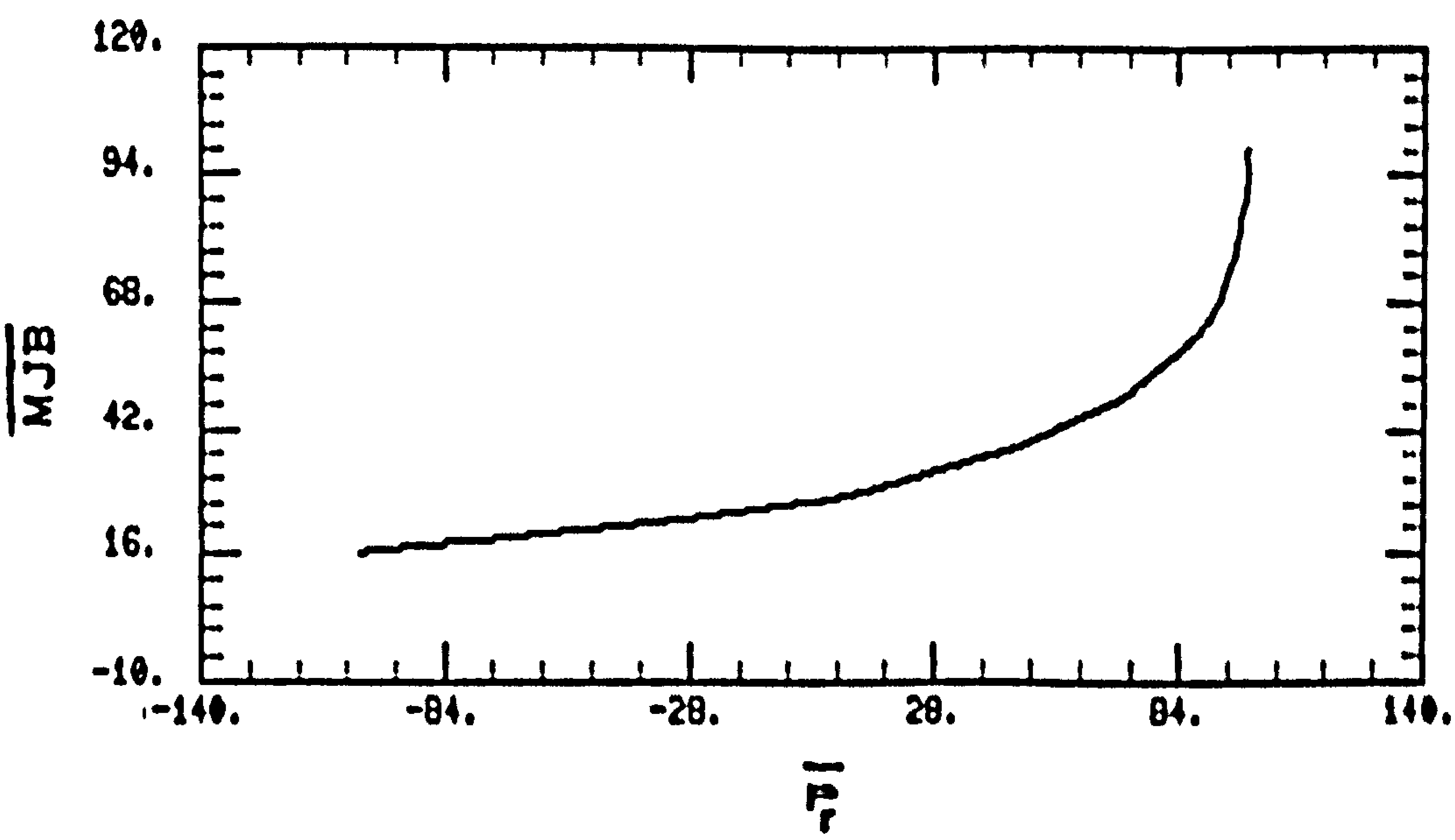


Figure 6.19

APPENDIX 6A

In this appendix the method used for solving the algebraic Riccati equation is outlined. The expressions obtained from analytically solving the LQ Problem formulation of system 2 are given by equations (6.44) through (6.47). For convenience these equations are rewritten here as:

Optimal state feedback controller:

$$u(t) = -Kx(t) \tag{6A.1}$$

where,

$$K = R^{-1}B^{T}P \tag{6A.2}$$

Steady state Riccati equation:

$$A^{T}P + PA - PBR^{-1}B^{T}P + Q = 0 \tag{6A.3}$$

Minimum objective function:

$$MJ = x_{o}^{T}Px_{o} \tag{6A.4}$$

Clearly, the determination of the optimum controller matrix, K, and the minimum objective function relies on the solution of the matrix Riccati equation. A number of methods for solving this equation are available. A review of these methods is given by Anderson and Moore [1971]. One approach on which the simple iteration algorithm used in this study is based is the Kleiman's [1968] technique. Using equations (6A.2) and (6A.3) it can be shown that:

$$(A-BK)^T P + P(A-BK) = -K^T R K - Q \tag{6A.5}$$

Kleiman's method is an iterative process which involves the simultaneous solution of equations (6A.2) and (6A.5).

<u>Algorithm</u>

Step 1. Choose any matrix K_m for which $(A-BK_m)$ is a stability matrix, i.e the eigenvalues of $(A-BK_m)$ should have negative real parts. Where m=1.

Step 2. Solve equation (6A.5) for the symmetric matrix P_m. This is a Liapunov type equation for which there exist several methods of solution. Four different approaches have been given by Rothschild and Jameson [1970] of which the reliable algorithm 1 has been used here.

Step 3. Set $K_{m+1} = R^{-1}B^T P_m$

Step 4. Check for convergence

(a) calculate

$$AE = \Sigma \left| K_{m+1}(i,j) - K_m(i,j) \right| \quad \forall\ i,j$$

(b) if $AE < \epsilon$ terminate. Otherwise set m=m+1 and go to step 2. Where ϵ is a convergence tolerence and K(i,j) is the (i,j)th element of the controller matrix K.

This algorithm has been implemented in the form of a computer program which uses the Digital Equipment Corporation (DEC) library of matrix operation subroutines described in DEC Scientific Subroutines Programmer's Reference manual, AA-1101D-TC, october 1981. This program, which is given under the name "SRECCA" in the software appendix, also computes the minimum value of the objective function.

A convergence tolerence, ϵ , of 0.001 has been employed.

CHAPTER 7

INTEGRATED DESIGN AND CONTROL OF A BINARY DISTILLATION COLUMN

7.1 Introduction

The importance of distillation in the chemical and petrochemical industries is well known. Distillation columns are not only significant components of the overall capital costs, but also require a large amount of the energy used and hence dominates the operating costs of the plant. In the face of rising energy and raw material costs the urge for operating these columns efficiently has increased considerably. A column operates efficiently only if it has been well designed and it is controlled effectively. This suggests that the design of the column and that of its control system should be considered simultaneously.

In this chapter the integrated design and control of an industrially important binary distillation column, namely an n-butane--isobutane splitter, is considered. The proposed design algorithm, see section 3.2, is used for such an activity.

The chapter is structured as follows. The steady state and dynamic behaviour of binary distillation columns can be represented by a large number of models of varying degrees of complexity. Section 2 and 3, respectively, are concerned with those steady state and dynamic models we have used.

The system (column and its control system) to be designed is defined in section 4. In section 5 the criteria used for ranking the large number of feasible designs are treated in some detail. The actual design of the n-butane--isobutane splitter is carried out in section 6.

7.2 Steady state modeling

The design of distillation columns is carried out using steady state models of varying degrees of complexity. It goes without saying that such a complexity is dictated by the nature and number of assumptions introduced. The static equations describing a binary distillation column, which have been used in this study, are given below. The assumptions required for their development are:

(a) Constant molal overflow

(b) The feed is saturated liquid

(c) A total condenser is used

(d) Murphree efficiency determines vapour composition.

(e) Constant relative volatility

(f) Negligible heat losses from the column

(g) Constant pressure

The following symbols are used:

F feed rate (saturated)

D distillate flow rate

B bottoms flow rate

V vapour flow rate

L liquid flow rate in the rectifying section

L_S liquid flow rate in the stripping section

X_F feed composition

X_D distillate composition

X_B bottom product composition

N_T total number of trays including a partial reboiler and a total condenser

Y_n composition of the vapour leaving tray n; $n=1,2,3,\ldots,N_T-1$. 1 denotes the reboiler and N_T denotes the condenser.

X_n composition of the liquid leaving tray n; $n=2,3,\ldots,N_T$.

R_m minimum reflux ratio

N_m minimum number of theoretical trays.

α relative volatility

R reflux ratio

N_F feed tray

All flow rates are in (Kmoles/hr) and all compositions are given as mole fractions.

Overall material balances:

column:

$$F = D + B \tag{7.1}$$

condenser:

$$V = L + D \tag{7.2}$$

reboiler:

$$L_s = V + B \tag{7.3}$$

component material balances:

overall:

$$FX_F = DX_D + BX_B \tag{7.4}$$

stripping section:

$$VY_n = L_s X_{n+1} - BX_B; \qquad n=1,2,\ldots\ldots,N_F-1 \tag{7.5}$$

feed stage:

$$VY_n = FX_F + LX_{n-1} - DX_D; \qquad n=N_F \tag{7.6}$$

rectifying section:

$$VY_n = LX_{n+1} + DX_D; \; n=N_F+1,N_F+2,\ldots\ldots,N_T-1 \tag{7.7}$$

Equilibrium relationships:

Actual tray:

$$Y_n = \frac{E_m \alpha X_n}{1+(\alpha-1)X_n} + (1-E_m)Y_{n-1}; \qquad n=2,3,\ldots\ldots,N_T-1 \tag{7.8}$$

where E_m is the Murphree stage efficiency (constant).

Ideal reboiler:

$$Y_1 = \frac{\alpha X_B}{1+(\alpha-1)X_B} \tag{7.9}$$

Reflux ratio:

$$R = L/D \tag{7.10}$$

Total condenser:

$$Y_n = X_D; \quad n=N_T-1 \tag{7.11}$$

$$X_n = X_D; \quad n=N_T \tag{7.12}$$

Minimum reflux ratio, Underwood [1948]:

$$R_m = \frac{1}{(\alpha-1)}\left[\frac{X_D}{X_f} - \frac{\alpha(1-X_D)}{(1-X_f)}\right] \tag{7.13}$$

Minimum number of theoretical trays, Fenske [1932]:

$$N_m = \frac{1}{\ln(\alpha)} \ln\left[\frac{X_D(1-X_B)}{X_B(1-X_D)}\right] \tag{7.14}$$

There are $\{15+2(N_T-1)\}$ design variables, which are listed in the above symbol table, and $\{9+2(N_T-1)\}$ independent equality constraints, equations (7.1) through (7.14). Hence, to completely define the system of equations describing the column, the values of six independent variables have to be chosen a priori. In most cases, the values of the majority of these degrees of freedom are dictated by some technical, enviromental or economic constraints. The remaining free variables are usually selected such that a cost or profit function is optimized. Here, however, we are interested in selecting their values such that the best design is obtained. A vector of criteria, in lieu of a single performance index, is used to judge the different feasible designs. This vector contains measures of the steady state costs as well as the dynamic behaviour of the operating column. The set of the six design variables which are, usually, either preselected or adjusted during the design process include the feed rate, F, the feed composition, X_F, the distillate composition, X_D, the reflux ratio, R, the feed tray, N_F, the relative volatility, α , and the bottom product composition, X_B.

Equations (7.1) through (7.14) can be solved using a stage-to-stage approach which is computationally equivalent to the McCabe-Thiele graphical procedure. An algorithm based on this approach, which has been described by Buckley et al. [1978], is used in this work. This approach has two drawbacks, one of which is that the required computation time is proportional to the number of trays. The other limitation is related to the fact that the number of trays must be an integer number which leads to the violation of the top or bottom product specifications. To allow for this latter shortcoming of the method, an iterative process wherein one of the free variables, which is usually the reflux ratio, is continuously readjusted until a certain convergence tolerence is satisfied. Two of the many possible convergence procedures were reported by Buckley et al. [1978]. These are a simple proportional controller technique and the 'projection' method of Wegstein [1958]. Tests have been carried out using these two methods with the latter being found to exhibit very fast convergence. However, we have not used these convergence techniques in this design exercise since the distillation sizing algorithm has been incorporated in an optimization package which in itself is an iterative process yielding an optimum design with product purities which exactly match the product specifications.

A number of other techniques are available for solving the steady state models of binary or pseudo-binary distillation colums. Some of these approaches are suitable for simple models only whereas others have been devised to tackle models of high degree of complexity. They include graphical, analytical and shortcut design methods; Most of which are treated in the books of King [1980], Henley [1980] and Calo et al. [1981]. A recent paper by Haskins et al. [1985] provides a review and a comparison of the majority of the available group (shortcut) methods which are very useful for online computer calculations.

The analytical equation of Smoker [1938] is another suitable method for solving steady state models of the type given by equations (7.1) through (7.14) to yield an exact solution. It assumes, however, that the trays are ideal (or 100% efficient). This difficulty can be overcome by using the efficiency to modify the vapour-liquid equilibrium relationship such that a pseudo-relative volatility is obtained. Compared to the tray-to-tray approach, The Smoker's equation yields a quick answer and the solution time required is independent of the number of trays. However, the latter has the disadvantage that it does not provide individual stage compositions which might be needed for further calculations such as the estimation of the column's dynamics. We have also used the Smoker equation for preliminary studies.

7.3 Dynamic modeling

The proposed plant design algorithm may involve the comparison of the steady state and transient performance of a large number of feasible solutions. Therefore, what is required is an approximate unsteady state model which gives a reasonably good prediction of the column dynamic behaviour in a short period of time. Approximate models describing the dynamic behaviour of binary distillation columns have been developed by many workers. The majority of these models have been compared by Moliis-Mellberg

[1974] and Waller [1979]. They include:

(a) Robinson and Gilliland [1950]

(b) Armstrong and Wilkinson [1957]

(c) Williams and coworkers [1965-1972]

(d) Wahl and Harriott [1970]

(e) Waller [1979]

The authors have concluded that models (a) and (b), though simple, are not very accurate. Although model (c) is similar in concept to models (d) and (e), it is limited to predicting the response of the reboiler and condenser to changes in the feed composition and reflux flow rate. Only models (d) and (e), which have been found to be of comparable accuracy, are suitable for predicting the response of all trays to the common forcing functions. Both models rely on a few parameters which are calculated from the steady state data. The advantage of Wahl and Harriott model over that of Waller is that the column time constants can be obtained directly from the given graphical correlations. Also mathematical models may be fitted to these graphs which can then be used for routine or computer calculation. This, in turn, facilitates the use of these time constants in an iterative approach if desired. For these reasons Wahl and Harriott's model has been chosen for this study. Waller's model is given in the form of frequency response curves from which the column transfer function matrix can be extracted.

7.3.1 Simplified full order model

Wahl [1967], and Wahl and Harriott [1970] used a linearised full order model, namely the Constant Molal Overflow (CMO) model, to study and analyse the behaviour of binary distillation columns which led to the development of their approximate model. The CMO model is based on a large number of simplifying assumptions which include:

(a) Negligible vapour holdup

(b) Liquid on a tray is perfectly mixed

(c) Constant Molal Overflow (constant vapour and liquid rates throughout the column)

(d) Fast enthalpy and mass accumulation

The equations which describe the column dynamics are:

Component material balance:

Reboiler:

$$\frac{d}{dt}(H_1X_B) = L_sX_2-VY_1-BX_B \tag{7.15}$$

Stripping section:

$$\frac{d}{dt}(H_nX_n) = L_s(X_{n+1}-X_n) + V(Y_{n-1}-Y_n);$$

$$n = 2,3,\ldots\ldots,N_F-1. \tag{7.16}$$

Feed tray:

$$\frac{d}{dt}(H_nX_n) = F(X_F-X_n) + L(X_{n+1}-X_n)$$

$$+ V(Y_{n-1}-Y_n); \quad n=N_F \tag{7.17}$$

Rectifying section:

$$\frac{d}{dt}(H_nX_n) = L(X_{n+1}-X_n) + V(Y_{n-1}-Y_n);$$

$$n=N_F+1, N_F+2, \ldots\ldots, N_T-1. \tag{7.18}$$

Total condenser (a perfectly mixed tank):

$$\frac{d}{dt}(H_nX_D) = V(Y_{n-1}-X_D); \quad n=N_T \tag{7.19}$$

In the preceeding equations H_n denotes the holdup of tray n.

The other relationships describing the behaviour of the column are the algebraic overall material balances, equations (7.1) through (7.3), and the algebraic equilibrium relationships, equations (7.8) and (7.9).

The CMO model is the simplest full order model which can be used to describe the dynamics of a distillation column. A comprehensive model is the one which uses composition, holdup and enthalpy as the state variables. Many other models of varying degrees of complexity can be found in the literature. A good review of these models and of the different approaches used for reducing them to obtain simpler models is given by Howell [1985].

7.3.2 Wahl and Harriott model

Wahl and Harriott [1970] studied the transient response of tray composition in binary distillation columns described by linearised CMO models. Four loads were considered:

(a) Feed rate*, f

(b) Feed composition, x_F

(c) Boilup rate, v

(d) Reflux rate, ℓ

They found that the response of a column to any of these upsets can be characterised by two parameters. A time constant, T_s, obtained by assuming that the product streams are dependent on the column average concentration only, and a reduced circulation rate, L_R, which represents the extent to which the column is maintained at equilibrium and hence the extent of the validity of the assumption introduced in obtaining T_s. A table of equations required for the calculation of the column steady state gains and T_s has been given by the authors. Due to the fact that this table contains a couple of errors, it has been corrected and is

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* Throughout this chapter column flow rates and compositions denoted by small letters are perturbation variables.

reproduced in appendix 7B. L_R is defined as:

$$L_R = \frac{T_S L}{H_T} \tag{7.20}$$

where H_T is the total column holdup.

At very high L_R, the column responds, to any of the four loads, as a first order lag with a time constant approximately equal to T_S. The type of response becomes more dependent on the particular applied input as the reduced circulation rate approaches zero. For the intermediate region between these two extreme cases, Wahl and Harriott recomended the use of the following transfer functions:

$$\frac{x_n(s)}{x_F(s)} = \frac{k_p(T_z s+1)}{(T_1 s+1)(T_3 s+1)} \tag{7.21}$$

$$\frac{x_n(s)}{\ell(s)} = \frac{k_p}{(T_1 s+1)} \tag{7.22}$$

$$\frac{x_n(s)}{v(s)} = \frac{k_p}{(T_1 s+1)} \tag{7.23}$$

$$\frac{x_n(s)}{f(s)} = \frac{k_p}{(T_1 s+1)} \quad ; \quad n<N_F \tag{7.24}$$

$$\frac{x_n(s)}{f(s)} = \frac{k_p(T_z s+1)}{(T_1 s+1)(T_2 s+1)} \quad ; \quad n>N_F \tag{7.25}$$

where $x_F(s)$, $x_n(s)$, $\ell(s)$, $v(s)$ and $f(s)$ are the Laplace transform of perturbations in the feed composition, plate n composition, the reflux rate, the vapour rate and the feed rate respectively. k_p refers to the plant steady state gain, the value of which is, of course, dependent on the input and output variables in question.

Graphical correlations, which relate the dynamic parameters of these transfer functions to T_s and L_R, are given by the authors. In this work, mathematical models have been fitted to these curves using the statistical subroutines package of Digital Equipment Corporation (see the Scientific Subroutines Programmer's Reference Manual, AA-1101D-TC, october 1981) and the E02CAF routine of the NAG library mark 11 version. These models facilitate and permit the calculation of the column time constants online so that, if desired, they can be easily incorporated in an iterative process. The following models represent the full range of Wahl and Harriott curves unless otherwise stated.

Principal (first) time constant, T_1:

$$b = -0.028a^2 + 0.112a + 0.891 \tag{7.26}$$

where,

$$a = \log(L_R)$$

$$b = T_1/T_s$$

Second time constant, T_2:

Linear range:

$$c = 0.469a + b - 0.751 \tag{7.27}$$

where,

$a = \alpha$

$b = \log(L_R), \qquad L_R \geqslant 6$

$c = \log(T_S/T_2)$

Full range:

$$c = \sum_{i=1}^{3} \sum_{j=1}^{2} X_{ij} f_{i-1}(b^*) f_{j-1}(a^*) \tag{7.28}$$

where,

$f_m(x) = \cos\{m\cos^{-1}(x)\} \qquad m=1,2,3,\ldots$ is the Chebyshev polynomial of the first kind.

$a^* = (2a-3.75)/1.25, \qquad -1 \leqslant a^* \leqslant 1$

$b^* = (2b-1.18)/2.22, \qquad -1 \leqslant b^* \leqslant 1$

$a = \alpha$

$b = \log(L_R)$

$c = \log(T_S/T_2)$

$$X = \begin{bmatrix} 0.908 & 0.188 \\ 0.805 & 0.160 \\ 0.149 & -0.040 \end{bmatrix}$$

Third time constant, T_3:

$$c = 1.20a + 0.023b - 0.603 \tag{7.29}$$

where,

$a = \log(N_T - 2)$

$b = R$

$c = \log(VT_3/H_p)$

Subscript p denotes a plate

Fourth time constant, T_4:

$$b = 1.47a - 0.993 \tag{7.30}$$

where,

$a = \log(N_T - 2)$

$b = \log(VT_4/H_p)$

Zero, $1/T_z$:

$$b = 6.14a^4 - 6.66a^3 + 2.74a^2 - 0.13a - 1.0, \quad 0 < a \leqslant 0.68 \tag{7.31}$$

where,

$$a = \frac{0.5H_i}{\{H_i+H_p(N_T-N_F-1)\}} \quad ; \qquad i=N_T \quad \text{for } x_D$$

as the output variable, Wahl [1967].

$$a = \frac{(H_i-H_p(n-N_T+\frac{1}{2}))}{\{H_i+H_p(N_T-N_F-1)\}} \quad ; \qquad i=N_T \quad \text{for } x_n \text{ as}$$

the output variable.

$$b = \frac{T_z-T_2}{T_z+T_4}$$

All of the above models fit the correlations of Wahl and Harriott within the limitation of the scatter of the original data.

7.4 Design problem

The design data and system constants for the considered n-butane--isobutane splitter are given in table 7.1 below. Note that isobutane is the more volatile component and hence it is removed at the top end of the column.

These design data and system constants have been obtained from a number of sources which include Happel and Jordan [1975], Shinskey [1984], Perry and Chilton [1973], and Reid and Sherwood [1966]. In addition to these design data assume that it is desired to produce a distillate which is 95% or more isobutane and a bottom product which 10% or less isobutane, i.e

$$X_D \geqslant 0.95 \tag{7.32}$$

and

$$X_B \leqslant 0.10 \tag{7.33}$$

Table 7.1 Design data and system constants

X_F=0.5,	F=1.0,	α=1.35,	E_m=1.0,	e_l=548.5,	e_g=11.135,
T=38,	P=4.9, U=2044,		T_{lm}=16.5,	v_g=2196,	T_{wi}=26.5,
T_{wo}=46,	C_{pw}=4.19,	M_w=58,	h_d=17523.0,	h_s=2091	

Terms not already defined have the following meanings:

- U — overall heat transfer coefficient in either the reboiler or condenser, Kj/(hr)(m^2)(^oC)
- P — column pressure, atm
- e_g — vapour density at feed tray, kg/m^3
- e_l — liquid density at feed tray, kg/m^3
- v_g — boilup superficial velocity, m/hr
- T — feed tray temperature, ^oC
- T_{lm} — log mean temperature difference in either reboiler or condenser, ^oC
- T_{wi} — inlet temperature of cooling water, ^oC
- T_{wo} — outlet temperature of cooling water, ^oC

C_{pw} heat capacity of water, $Kj/_{l}.^{o}C$

M_w molecular weight of n-butane/isobutane

h_d latent heat of vapourisation of the liquid stream at feed plate, Kj/Kmole

h_s latent heat of vapourisation of steam, Kj/kg

The operating splitter is to be controlled using a scheme in which, both, the top and bottom products compositions are to be kept at their respective design values. Such a control approach is referred to as dual composition control or two-point control. The use of dual composition control reduces the energy required to achieve a specified separation and hence a reduction in the operating costs. In addition, the control of both compositions reduces the concentration load disturbances on the downstream plant units.

A large number of papers on two-point control have been published. A comprehensive review is given by Waller [1981]. The monograph by McAvoy [1983a], and the recent paper by McAvoy and Wang [1986] can be consulted for additional literature which appeared after 1981.

Depending on the manipulated variables used, many dual composition control schemes are possible. A simple scheme is the popular conventional control method in which changes in vapour boilup are used to control the bottoms composition and changes in the reflux rate are used to control the distillate composition. This control approach is also referred to as the energy balance scheme since L and V (energy balance variables) are used as the manipulated variables. As indicated in the proposed design algorithm, the choice of the control system can be relegated until the static and/or dynamic characteristics of the design which yields minimum steady state costs are analysed. However, in this study we assume that the simple energy balance control scheme is chosen a priori as the most suitable scheme for the control of the n-butane--isobutane splitter. Some of the factors which influence the choice of a particular scheme for the dual composition control of a given column include simplicity, the amount of interaction, the likelihood of the manipulated variables saturation and system integrity.

Another simple control structure for two-point control is the material balance scheme, proposed by Shinskey [1969], in which the top product composition is controlled through manipulation of the distillate flow rate (material balance variable) and the vapour flow rate is used to control the bottoms composition. One major drawback of this scheme is that if the $D-X_D$ loop fails the dynamic performance of the the column in question will deteriorate considerably. Resetting the controller parameters of the other loop will not lead to any significant improvements, Weischedel [1981], and Tolliver and Waggoner [1980]. The energy balance scheme does not suffer from such a drawback.

In terms of the amount of interaction it is very difficult to choose between the energy and material balance schemes. Using the Bristol Number (BN), which is defined in subsection 7.5.3 below, Shinskey [1979] showed that for a step change in one of the two loops, a system with a BN of 0.5, which is an indication of very strong interaction for material balance schemes, exhibits a better transient performance than a system with a BN of 2. For a disturbance upset the opposite result has been obtained by Stanley et al. [1985]; a system with a BN of 38, which is an indication of high interaction for an energy balance scheme, was found to outperform a system with a BN of 0.44.

Feed rate and composition changes are, usually, the major disturbances affecting a distillation column. Of the two, the feed rate upsets are much greater in both frequency and magnitude. In this study we assume that changes in composition, if any, are filtered out before the n-butane--isobutane mixture enters the column. Therefore, the column control system will have to deal mainly with variations in the feed rate.

Thus using the recommendations of Wahl and Harriott [1970], the considered design example can be represented by the following transfer function matrix:

$$\begin{bmatrix} x_D(s) \\ x_B(s) \end{bmatrix} = \begin{bmatrix} g_{11}(s) & g_{12}(s) \\ g_{21}(s) & g_{22}(s) \end{bmatrix} \begin{bmatrix} \ell(s) \\ v(s) \end{bmatrix} . \begin{bmatrix} g_{f1}(s) \\ g_{f2}(s) \end{bmatrix} f(s) \qquad (7.34)$$

where,

$$g_{11}(s) = \frac{k_{11}}{T_1 s+1} \tag{7.35}$$

$$g_{12}(s) = \frac{k_{12}}{T_1 s+1} \tag{7.36}$$

$$g_{21}(s) = \frac{k_{21}}{T_1 s+1} \tag{7.37}$$

$$g_{22}(s) = \frac{k_{22}}{T_1 s+1} \tag{7.38}$$

$$g_{f1}(s) = \frac{k_{f1}(T_z s+1)}{(T_1 s+1)(T_2 s+1)} \tag{7.39}$$

$$g_{f2}(s) = \frac{k_{f2}}{T_1 s+1} \tag{7.40}$$

The column model as given above does not include the dynamic characteristics of the composition measuring devices. Chromatographs and online analysers are known to introduce dead times in the range of 2 to 30 minutes, Fuentes and Luyben [1983]. Using a time delay of 5 minutes to model the composition measuring elements, the complete block diagram of the considered system is as given in figure 7.1.

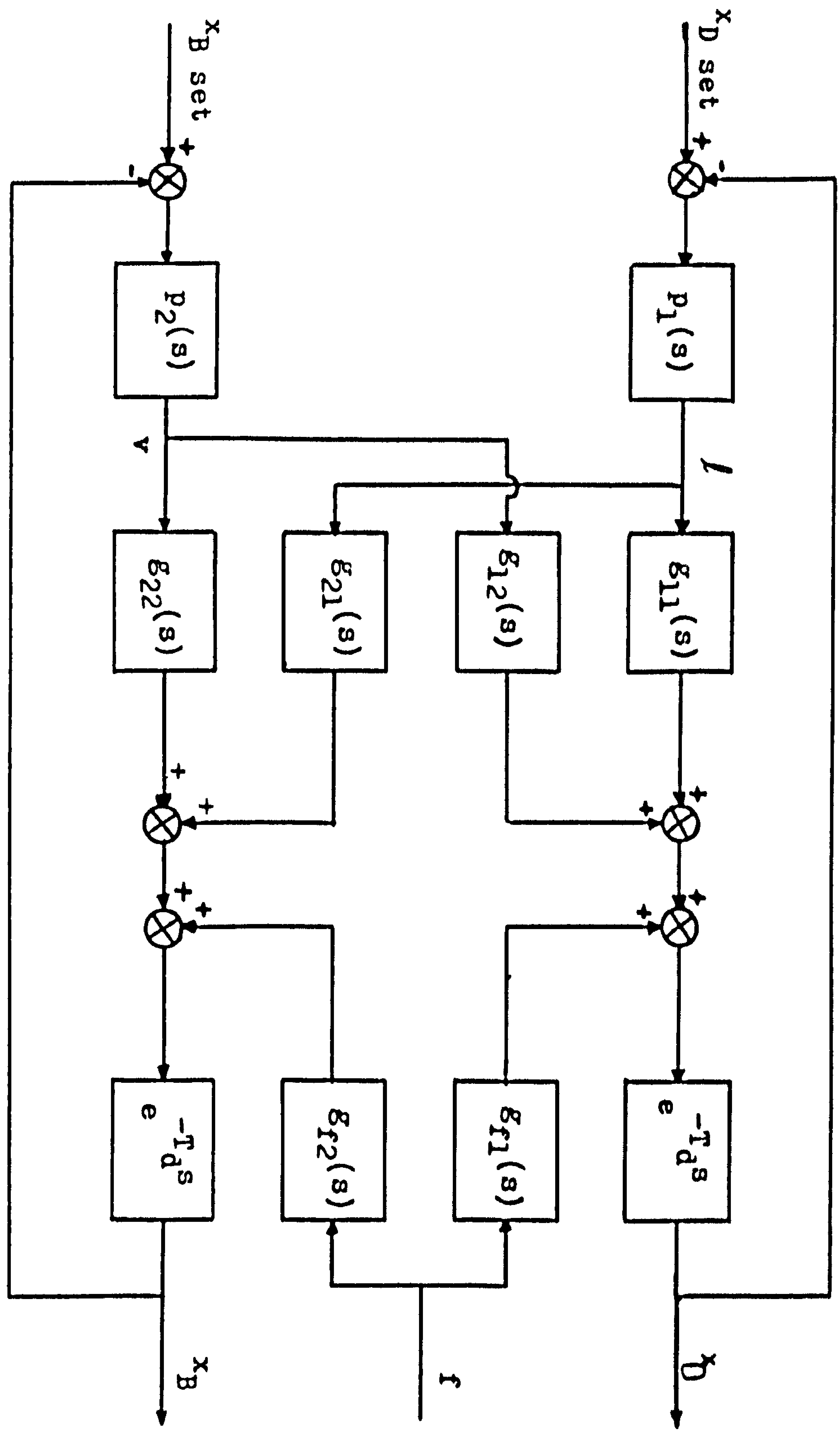

Figure 7.1 System

7.5 Design criteria

Four measures, which include the total steady state cost, the Bristol number and the two steady state gains, k_{f1} and k_{f2}, relating the top and bottom product compositions to changes in the feed rate, are used here as the design criteria. The static cost is a measure of economic performance - in the steady state sense - of the column whereas the other three criteria are related to the column degree of controllability. The Bristol number is a measure of the expected interaction between the two control loops and the sensitivity of the plant to modeling errors. k_{f1} and k_{f2} are measures of the sensitivity of the controlled variables, x_D and x_B, to variations in the feed rate.

7.5.1 Cost function

The cost function we have used has the form:

Total cost = capital charges + operating costs

Capital charges:

Column (trays + shell):

$$C_c = C_1 S(N_T-2)/E_m \tag{7.41}$$

where,

C_1 is the hourly incremental unit investment cost, $\$/(m^2)(plate)(hr)$

S is the tower cross-sectional area, m^2

C_c is the cost of the column, \$/hr

Since the column cross-sectional area is given by:

$$S = \frac{VM_w}{v_g e_g} \tag{7.42}$$

C_c can be written as:

$$C_c = B_1(N_T-2)V \tag{7.43}$$

where B_1 is given by:

$$B_1 = \frac{C_1 M_w}{v_g e_g E_m} \tag{7.44}$$

Reboiler and condenser:

The combined condenser and reboiler costs, C_{rc}, can be written as:

$$C_{rc} = C_2(A_R+A_C) \tag{7.45}$$

where,

C_2 is the hourly incremental unit investment cost of reboiler and condenser, \$/(m^2)(hr)

A_r is the heat transfer area of the reboiler, m^2

A_c is the heat transfer area of the condenser, m^2

Assuming the heat absorbed from the reboiler and the heat transfered into the condenser to be equal, we have:

$$Q_h = UT_{1m}(A_r+A_c) \tag{7.46}$$

and

$$Q_h = 2h_dV \tag{7.47}$$

where Q_h is the combined heat transfered into the condenser and the heat absorbed from the reboiler.

Equations (7.46) and (7.47) yield:

$$(A_r+A_c) = \frac{2h_dV}{UT_{1m}} \tag{7.48}$$

Substituting this expression for (A_r+A_c) into equation (7.45) gives:

$$C_{rc} = B_2V \tag{7.49}$$

where B_2 is given as:

$$B_2 = \frac{2C_2h_d}{UT_{1m}} \tag{7.50}$$

Operating costs:

Utilities costs:

The cost of cooling water and steam, C_u, is:

$$C_u = B_3 V \tag{7.51}$$

where B_3 is the combined cost of the coolant and steam required to condense and vapourise, respectively, 1 Kmole of vapour.

These simple models for estimating the capital and utilities costs of distillation columns are similar to those developed by Colburn [1943] and discussed in much more details by Happel and Jordan [1975].

Product losses:

Shinskey [1984] used the following model for calculating the cost, C_{pl}, associated with the product losses.

$$C_{pl} = B_4 B X_B + B_5 D(1-X_D) \tag{7.52}$$

where B_4 is the cost penalty for loosing isobutane in the bottom product and B_5 is the penalty for loosing n-butane in the top product.

The total cost function is the sum of equations (7.43), (7.49), (7.51) and (7.52).

$$C_T = B_1(N_T-2)V+B_2V+B_3V+B_4BX_B+B_5D(1-X_D) \qquad (7.53)$$

7.5.2 Steady state gains

A procedure for calculating the steady state gains relating the liquid composition on a tray to a given load, k_p in equations (7.21) through (7.25), is given by Wahl and Harriott [1970]. The loads considered by the authors are the feed composition, the feed rate, the reflux rate, the boilup rate, and the simultaneous reflux and boilup rates. The method involves the linearisation of the CMO dynamic model of the column and setting its derivatives to zero. By manipulating the resulting set of algebraic equations, they obtained a simpler set of relationships which is suitable for computer or routine calculation. These equations are reproduced in appendix 7B.

An approach for obtaining quick estimates of the steady state gains is to use an approximate analytical model of the column. Simple expressions for the column gains are developed by differentiating this model with respect to the load in question. This shortcut method is attractive because it is computationally much cheaper than the rigorous stage-to-stage approach of Wahl and Harriott. McAvoy [1983a] used the equation of Eduljee [1975], which is based on fitting a curve to Gilliland's [1940] graphical correlation, to develop expressions for the gains relating variations in X_D and X_B to a large number of loads.

However, the gains relating changes in the top and bottom product compositions to changes in the feed rate, $\partial X_D/\partial F$ and $\partial X_B/\partial F$, are not given by the author. The derivation of these gains is given in appendix 7C. Expressions for the gains relating changes in the top and bottom products compositions to changes in the feed rate are also included in this appendix. A number of column designs based on the n-butane--isobutane system have been used to compare for accuracy the column gains obtained using these simple expressions with the more rigorous and accurate approach of Wahl and Harriott. It has been found that in many cases, these expressions yield gains of low accuracy which suggests that they should only be used for rough estimates. In addition, these expressions are limited to giving the reboiler and condenser gains. However the approximate column time constant T_s, see section 7.3, requires the knowledge of the gains of all stages for its calculation. For these reasons, the method of Wahl and Harriott has been used throughout the design process of the n-butane--isobutane splitter.

7.5.3 Bristol Number (BN)

Interaction (or coupling) between control loops occurs when some or all of the manipulated variables in a given system affect more than one controlled variable. For distillation columns, control of both top and bottom products compositions may lead to strong interaction between the control loops. For a conventional two-point control scheme changes in vapour boilup affect the bottom composition as well as the distillate composition, while the reflux rate has an effect on the distillate and the bottoms compositions. It is well known that such interaction may have a detrimental effect on the closed loop behaviour of the column. The degree of performance deterioration is dependent on the strength of coupling.

The most widely used measure of interaction is the Relative Gain Array (RGA), which is also referred to as the Bristol Array, proposed by Bristol [1966]. Its popularity stems from the fact that it is easily computed and interpreted.

Consider the matrix G(0) of the plant steady state gains which is assumed to be square with elements k_{ij}, $(i=1,2,\ldots,m;\ j=1,2,3,\ldots,m)$. An element b_{ij} in the RGA, $\tilde{B}$, is the ratio of two steady state gains: The open loop gain between output y_i and input u_j when all the other loops are open to the open loop steady state gain between the same two variables y_i and u_j when all the other loops are closed with each loop containing at least one integrator. Mathematically, an element of the RGA can be expressed as:

$$b_{ij} = \frac{(\partial y_i/\partial u_j)_{u_p=0,\,p\neq j}}{(\partial y_i/\partial u_j)_{y_\ell=0,\,\ell\neq i}} \qquad (7.54)$$

The numerator of equation (7.54) is simply the (i,j)th element of G(0), i.e

$$(\partial y_i/\partial u_j)_{u_p=0,p\neq j} = k_{ij} \tag{7.55}$$

whereas the denominator is given by:

$$(\partial y_i/\partial u_j)_{y_\ell=0,\ell\neq i} = 1/\hat{k}_{ji} \tag{7.56}$$

where $\hat{k}_{ji}$ is the (j,i)th element of $G^{-1}(0)$.

This last result is obtained from the fact that $u=G^{-1}y$ and $(\partial u_j/\partial y_i)_{y_\ell=0,\ell\neq i} = \hat{k}_{ji}$.

Combination of equations (7.54) through (7.56) yield:

$$b_{ij} = k_{ij}\hat{k}_{ji} \tag{7.57}$$

For a (2x2) system b_{11} can be expressed in terms of the elements of G(0) as:

$$b_{11} = \frac{k_{11}k_{22}}{k_{11}k_{22}-k_{12}k_{21}} \tag{7.58}$$

b_{11} as defined by equation (7.58) is here referred to as the Bristol Number (BN). Due to the fact that the sum of the elements of each row and each column of the RGA is equal to one, property (b) below, for a (2x2) system the determination of the BN is all that is required for the Bristol array to be completely defined.

One limitation of the RGA is the fact that it is based on the steady state design data only. Hence for the cases where the interaction is strongly influenced by the plant dynamics, the RGA may not give the complete picture. Examples are given in the monograph on "Interaction Analysis. Principles and Applications" by McAvoy [1983a]. A second drawback of this measure is that it fails to indicate one way coupling which is, luckily, not exhibited by many industrial systems.

The following are the properties of the Bristol Array:

(a) It is invariant under scaling of the input and output variables.

(b) The sum of the elements of each row and each column of $\tilde{B}$ is equal to one.

(c) Any permutation of the rows and columns of G(0) results in the same permutation in $\tilde{B}$.

(d) For a (2x2) matrix G(0) whose elements are nonzero, the elements of $\tilde{B}$ are either all positive fractions or two elements greater than unity and two negative elements. The first case arises when G(0) contains an odd number of positive elements whereas the latter case occurs when G(0) has an even number of positive elements.

(e) An RGA equal to the unit matrix is obtained if G(0) is either diagonal (no interaction) or triangular which is the case of one way coupling referred to earlier.

(f) Large elements of the Bristol Array imply that the steady state gains matrix G(0) is nearly singular.

Property (f) suggests that there is a link between the RGA and the Condition Number (CN) of G(0). Indeed, recently Grosdidier et al. [1985] have analytically developed, for a (2x2) system, a relationship which relates the two measures.

$$K^*(G) = ||\tilde{B}||_1 + (||\tilde{B}||_1^2 - 1)^{1/2} \tag{7.59}$$

where K(G) is the condition number of matrix G(0). The condition number of a matrix G is given by equation (2.40) which is rewritten here for the l_2 -norm as:

$$K(G) = ||G||_2 . ||G^{-1}||_2 \tag{2.40a}$$

The astrisk denotes the optimum (minimum) condition number of the appropriately scaled matrix G. G is optimally scaled if pre- and postmultiplied by the diagonal matrices S_1 and S_2, respectively. Where,

$$S_1 = \begin{bmatrix} 1 & 0 \\ 0 & \left|\dfrac{k_{11}k_{12}}{k_{21}k_{22}}\right|^{\frac{1}{2}} \end{bmatrix} \tag{7.60}$$

and

$$S_2 = \begin{bmatrix} 1 & 0 \\ 0 & \left|\dfrac{k_{11}k_{21}}{k_{12}k_{22}}\right|^{\frac{1}{2}} \end{bmatrix} \tag{7.61}$$

A number of workers have extended the Bristol Array to include the effect of process dynamics. McAvoy [1983a] gives a comprehensive list of references. For (2x2) systems, one approach, defined by McAvoy [1983b], is to replace the steady state gains in equation (7.58) by their counterpart elements of G(s), i.e

$$b_{11}(s) = \frac{g_{11}(s)g_{22}(s)}{g_{11}(s)g_{22}(s) - g_{12}(s)g_{21}(s)} \tag{7.62}$$

A frequency dependent dynamic RGA is obtained by setting s=jw in equation (7.62). The frequency response of this dynamic measure of interaction can then be calculated. The author states that for a dynamic analysis of interaction to be necessary, two conditions must be satisfied:

(a) The RGA should change substantially with the frequency.

(b) The RGA at the ultimate frequency of one of the two loops should be substantially different from its steady state value. The second loop is opened when the ultimate frequency of the first loop is being estimated and vice versa.

In many systems, such as distillation, interaction is known to lead to performance deterioration in which case the coupling is said to be unfavorable. However, one can not generalise by saying that interaction is always unfavorable. Indeed, the question of how to determine whether interaction in a given system is favorable or unfavorable has been the concern of the control engineering community for quite sometime. Recently, Stanley et al. [1985] have proposed a very simple quantitative measure, Known as the Relative Disturbance Gain (RDG) for deciding if interaction in classical (2x2) PID control systems is favorable, in the steady state sense, or not. The RDG is dependent on the particular disturbance entering the system and is based on the steady state data only.

The system for which the RDG has been developed has exactly the same steady state structure as that shown in figure 7.1. Hence, this figure can be used for defining the elements of the RDG matrix without loss of generality.

The RDG element of the x_D-ℓ loop (loop 1), β_1 , is defined as the final change in the controller output ℓ that is required to counteract changes in f and bring x_D back to its set point when the x_B-v loop (loop 2) is under perfect steady state control divided by the same quantity for the case when loop 2 is open, i.e

$$\beta_1 = \frac{(\partial \ell/\partial f)_{x_D = x_B = 0}}{(\partial \ell/\partial f)_{x_D = v = 0}} \tag{7.63}$$

Setting s=0 in equation (7.34) the static model of the column is obtained:

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix} \begin{bmatrix} \ell \\ v \end{bmatrix} + \begin{bmatrix} k_{f1} \\ k_{f2} \end{bmatrix} f \qquad (7.64)$$

Using equations (7.63) and (7.64), β_1 is given as:

$$\beta_1 = b_{11} \left[1 - \frac{k_{f2} k_{12}}{k_{f1} k_{22}} \right] \qquad (7.65)$$

Similarly the RDG element of the x_B-v loop is:

$$\beta_2 = b_{11} \left[1 - \frac{k_{f1} k_{12}}{k_{f2} k_{11}} \right] \qquad (7.66)$$

A value of β_1 smaller than unity indicates that the change in controller output ℓ for the interacting system is less than that for the decoupled system which means that as far as loop 1 is concerned the static interaction is favorable.

For the case where equal importance is given to the performance of each of the two loops, the authors suggested that if the sum of the absolute values of the two individual RDG elements is less than two, i.e

$$|\beta_1| + |\beta_2| < 2 \qquad (7.67)$$

then the interaction present in the system is favorable.

It must be stressed that the RDG is dependent on the particular disturbance considered. If more than one load (including set point changes) enter the system, which is almost always the case, then the interaction is, most probably, unfavorable for some of the input disturbances. The authors have indicated that set point changes in one loop only always result in the interaction being highly unfavorable.

7.6 Integrated design

All optimization problems given in this section have been solved using the "complex" method described in chapter 4.

7.6.1 Minimum costs

Using equation (7.53) and the estimated cost factors given in appendix 7A, the total cost function becomes:

$$C_T = 2.6804\times10^{-4}(N_T-2)V + 2.060\times10^{-2}V + 2.2203\times10^{-2}V$$
$$+ 2.6652BX_B + 1.3282D(1-X_D) \qquad (7.68)$$

where C_T is the total costs in \$/hr.

Three (X_f, F, α) of the six possible degrees of freedom, see section 7.1, have been given as design data in table 7.1. This means that any three independent variables of the remaining $\{12+2(N_T-1)\}$ design variables can be chosen arbitrarily subject to the equality (steady state model) and inequality constraints of the problem. At this stage of the design process, we are interested in the values of these design variables which minimize the total cost function, equation (7.68). The reflux ratio, R, the distillate composition, X_D, and the bottom product composition, X_B, have been selected as these free variables since their specification renders the solution of the column steady state model a simple task.

The system inequality constraints are given by inequalities (7.32) and (7.33) which are rewritten as:

$$0.95 \leqslant X_D < 1.0 \tag{7.69}$$

$$0.0 < X_B \leqslant 0.10 \tag{7.70}$$

To avoid the possibility of obtaining non-realistic designs, the following additional inequality constraints have been used.

$$0.001 \leqslant R \leqslant 50 \tag{7.71}$$

$$1.0 < R/R_m \leqslant 100 \tag{7.72}$$

$$3 \leqslant N_T \leqslant 150 \tag{7.73}$$

The above upper bounds have been chosen realistically, yet large enough to ensure that a siginificantly large feasible region is explored.

A small set of randomly distributed feasible solutions has been generated using the FEASBL subroutine given in the software appendix at the end of this thesis. To provide some assurance that a global minimum has been found, a strategy which involves multiple optimization runs, each initiated at a different starting point chosen from these solutions, has been employed. The global minimum total cost has been found to be 0.2380 \$/hr. Most of the starting points used have converged to this solution. The characteristics of the optimum design are given in table 7.2. This design is also referred to as design A. When the starting point ($R=38.905$, $X_D=0.96601$, $X_B=0.09651$) has been used, it took the "complex" optimization algorithm a total number of 81 iterations to arrive at the optimal solution. Only those successful points, including the initial feasible points required to form the "complex", have been counted as iterations; that is when the worst point is replaced, by reflection, by a point that again has the highest total cost, that iteration is not counted. A plot of the total cost versus the number of iterations is given in figure 7.2. Notice the initially rapid convergence which is characteristic of the "complex" optimization method.

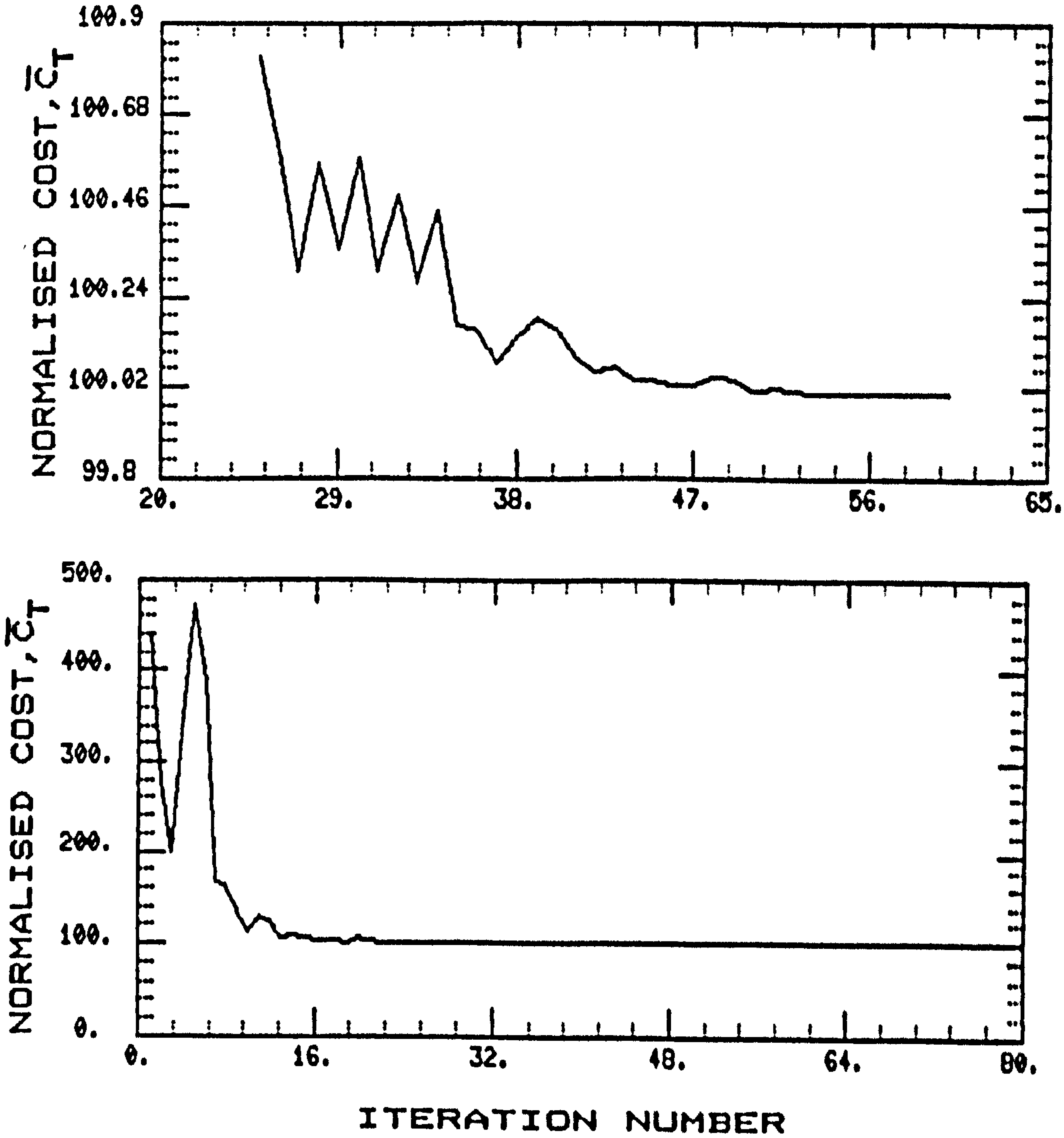

Figure 7.2 Normalised cost, $\bar{C}_T$, versus iteration number

$\bar{C}_T = (C_T/|0.238|)*100$

Optimization parameters:

Convergence tolerence = 1.0×10^{-6}
Number of points in the "complex" = 6
Reflection factor = 1.3

Table 7.2 Characteristics of design A

Design variables:	$R=5.9150$, $X_D=0.98448$, $X_B=0.00520$, $D=0.5053$, $B=0.4947$, $L=2.9888$, $V=3.4940$, $R_m=5.5055$, $N_m=32$, $N_T=78$, $N_F=42$.
dynamic parameters and plant gains:	$L_R=15.0$, $T_s=3.872$, $T_1=3.810$, $T_2=0.339$, $T_3=0.089$, $T_4=0.08$, $T_z=-0.0696$, $k_{11}=1.2880$, $k_{12}=-1.2568$, $k_{21}=0.6644$, $k_{22}=-0.6962$.
Design criteria:	$C_T=0.2380$, $b_{11}=14.5$, $k_{f1}=0.5418$, $k_{f2}=0.4468$.

The column holdups are required for the determination of its time constants. Ratios of vapour rate to holdups similar to those reported by Lenhoff and Morari [1982] have been used.

Tray holdup:

$$H_p = 1.45\times10^{-3}V \tag{7.74}$$

Condenser holdup:

$$H_i = 3.86\times10^{-2}V; \quad i=N_T \tag{7.75}$$

Reboiler holdup:

$$H_1 = 7.23\times10^{-2}V \tag{7.76}$$

In table 7.2, the relatively high value of L_R suggests that the minimum cost design will respond, to any of the inputs considered by Wahl and Harriott, approximately as a first order lag system with time constant T_s. This is clearly indicated by the small values of all column time constants other than T_1. The ratio of T_1 to T_s (0.984) is approximately equal to unity whereas that of T_2 to T_s (0.0876) is very small. The presence of a right half plane zero (negative T_z) in the column model suggests that inverse response will be exhibited by the column response to an upset in the feed rate. However, the fact that this zero is large means that its effects are negligible.

Using table 7.2, and equations (7.65) and (7.66) the sum of the absolute values of the two RDG elements is found to be 12.52. Since this value is greater than 2 the interaction present in the system is unfavorable to changes in the feed rate. A Bristol Number value of 14.5 means that design A will exhibit a considerable amount of interaction which will have a detrimental effect on the performance of the sought multiloop control system. In addition, this quantity indicates that the sensitivity of the system performance to modeling errors will be high. The minimum condition number, as given by equation (7.57), has a value of 56.1. Values of 0.5418 and 0.4468 for k_{f1} and k_{f2}, respectively, mean that the top and bottom products compositions will exhibit only moderate sensitivity to changes in the feed rate. For these reasons, we consider, at this stage, C_T and b_{11} to be primary criteria, and k_{f1} and k_{f2} to be secondary criteria.

At this point it is interesting to note that the Bristol number for the material balance control scheme discussed in section 7.5 has a value of 0.6 which is also an indication of strong interaction.

7.6.2 Minimum Bristol Number

The characteristics of the feasible design which has the lowest possible value of the BN are given in table 7.3. This design (also referred to as design C) has been obtained by solving the same optimization problem as for minimum total cost with b_{11} instead of C_T as the objective function. In this case, however, the feasible region has been further restricted by assuming that all designs whose cost exceeds that of design A by 20% or more to be highly undesirable, i.e. the additional inequality constraint:

$$C_T \leqslant 0.2856 \tag{7.77}$$

has been employed. Whenever possible, such constraints on costs should be imposed so as to reduce the number of nondominated solutions generated and hence reduce the effort required.

Table 7.3 Characteristics of design C

Design variables:	$R=5.1142$, $X_D=0.95494$, $X_B=0.01871$, $D=0.5141$, $B=0.4859$, $L=2.6291$, $V=3.1431$, $R_m=5.1092$, $N_m=24$, $N_T=116$, $N_F=61$.
Dynamic parameters and plant gains:	$L_R=5.2$, $T_s=1.729$, $T_1=1.655$, $T_2=0.433$, $T_3=0.155$, $T_4=0.139$, $T_z=-0.142$, $k_{11}=0.8913$, $k_{12}=-0.7495$, $k_{21}=0.9870$, $k_{22}=-1.1369$.
Design criteria:	$C_T=0.28556$, $b_{11}=3.70$, $k_{f1}=0.0112$, $k_{f2}=0.9786$.

An examination of tables 7.2 and 7.3 shows that if the total steady state cost is allowed to increase by 20% over its smallest possible value, a reduction of 74.5% (from 14.5 to 3.70) in the Bristol number can be obtained.

Compared to design A, design C exhibits much less interaction and much less sensitivity to modeling errors. The minimum condition number for design C has a value of 12.7. The steady state gain relating changes in the bottoms composition to changes in the feed rate has a much higher value for the minimum Bristol number design (k_{f2}=0.9786) than its counterpart for the minimum cost design (k_{f2}=0.4468). However, we assume that such a value is not large enough to call for the consideration of k_{f2} as a primary criterion. For design C, the sensitivity of the top product composition to variations in the feed rate is very low (k_{f1}=0.0112) and hence this criterion will be still considered as a secondary criterion. Therefore, the nondominated set is to be generated with C_T and b_{11} as the primary criteria, and k_{f1} and k_{f2} as the secondary criteria.

7.6.3 Nondominated set

The nondominated set of solutions is given in table 7.4 and figure 7.3. It has been generated according to the proposed design algorithm, section 3.2, with the total cost as the objective function and the Bristol number as the additional constraint to the set of inequalities defining the feasible region of the system. The cost minimization problem has been repeatedly solved using upper bounds on b_{11} of 12, 10, 8, 6, 5, and 4 to yield, respectively, solutions S2 through S7 in table 7.4. The secondary criteria values corresponding to this set of nondominated solutions are given in table 7.5 and plotted in figure 7.4. The overhead bar indicates that the criterion is normalised by dividing it by its absolute value at the minimum costs design and multiplying the result by 100, e.g $\bar{b}_{11}=(b_{11}/|14.5|)*100$.

An examination of figure 7.3 shows that three distinctive regions can be identified, two of which are characterised by the fact that large improvements in one primary criterion can be obtained at the expense of a small loss in the other. In the third region the conflict between the two criteria is relatively much more pronouced in the sense that significant improvements in one criterion can only be obtained at the expense of significant losses in the second criterion. The boundaries separating these regions are not fixed, and they are heavily dependent on the relative importance of the two primary criteria and on the designer himself. For the purpose of this study let us define these regions as:

region I: $\bar{C}_T \leqslant 100.55$

region II: $100.55 < \bar{C}_T < 109.0$

region III: $109.0 \leqslant \bar{C}_T$

Table 7.4 Nondominated set

solution (R, X_D, X_B)	$\bar{C}_T$	$\bar{b}_{11}$
S1 (5.9150,0.98448,0.00520)	100.00	100.0
S2 (5.7991,0.98130,0.00630)	100.17	81.0
S3 (5.7202,0.97903,0.00762)	100.55	67.6
S4 (5.5654,0.97593,0.00612)	101.58	54.1
S5 (5.5037,0.97640,0.00936)	103.52	40.9
S6 (5.4227,0.97430,0.00837)	106.03	34.4
S7 (5.2793,0.96630,0.01565)	113.18	27.7
S8 (5.1142,0.95494,0.01871)	120.00	25.5

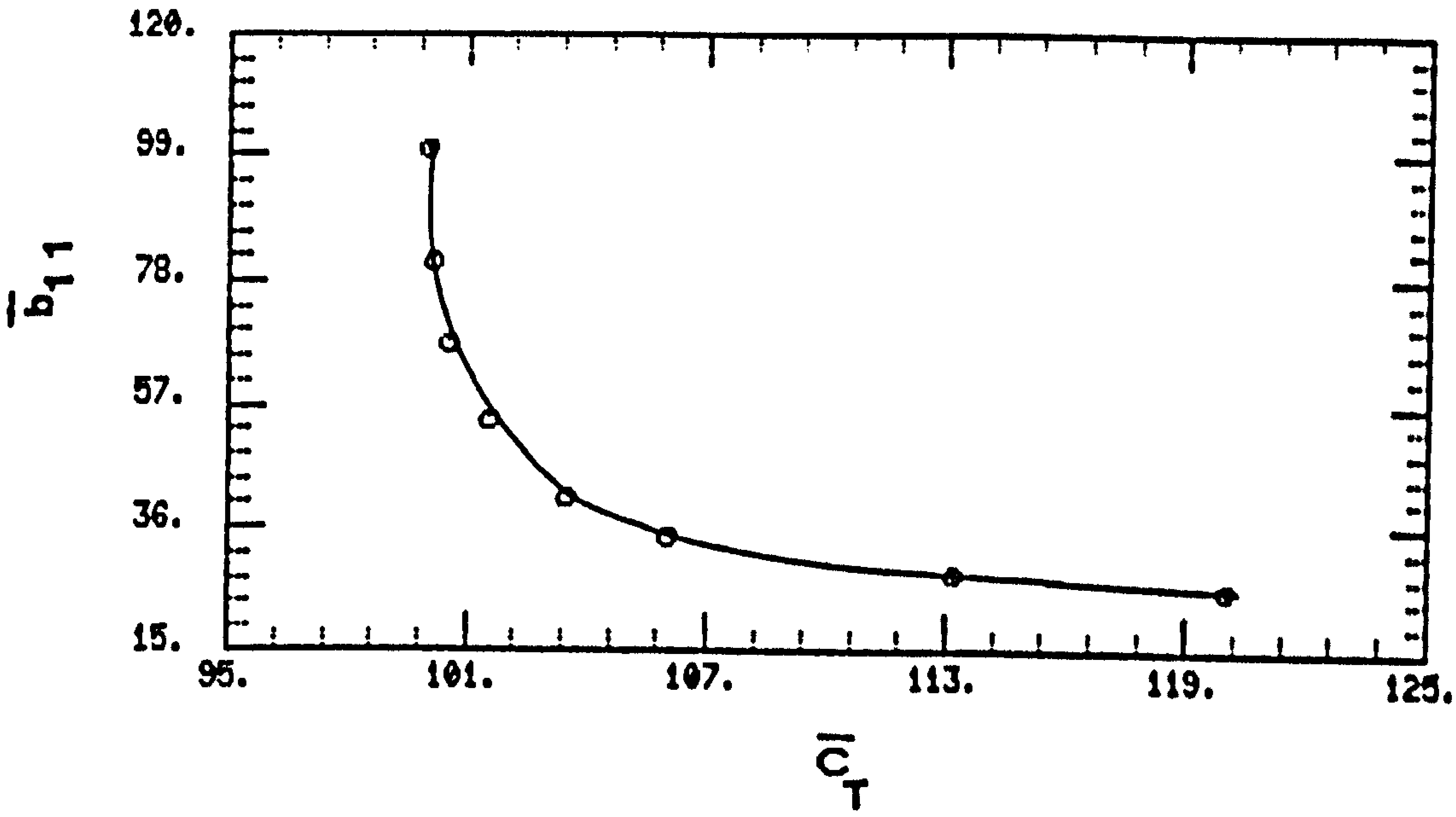

Figure 7.3 Nondominated set

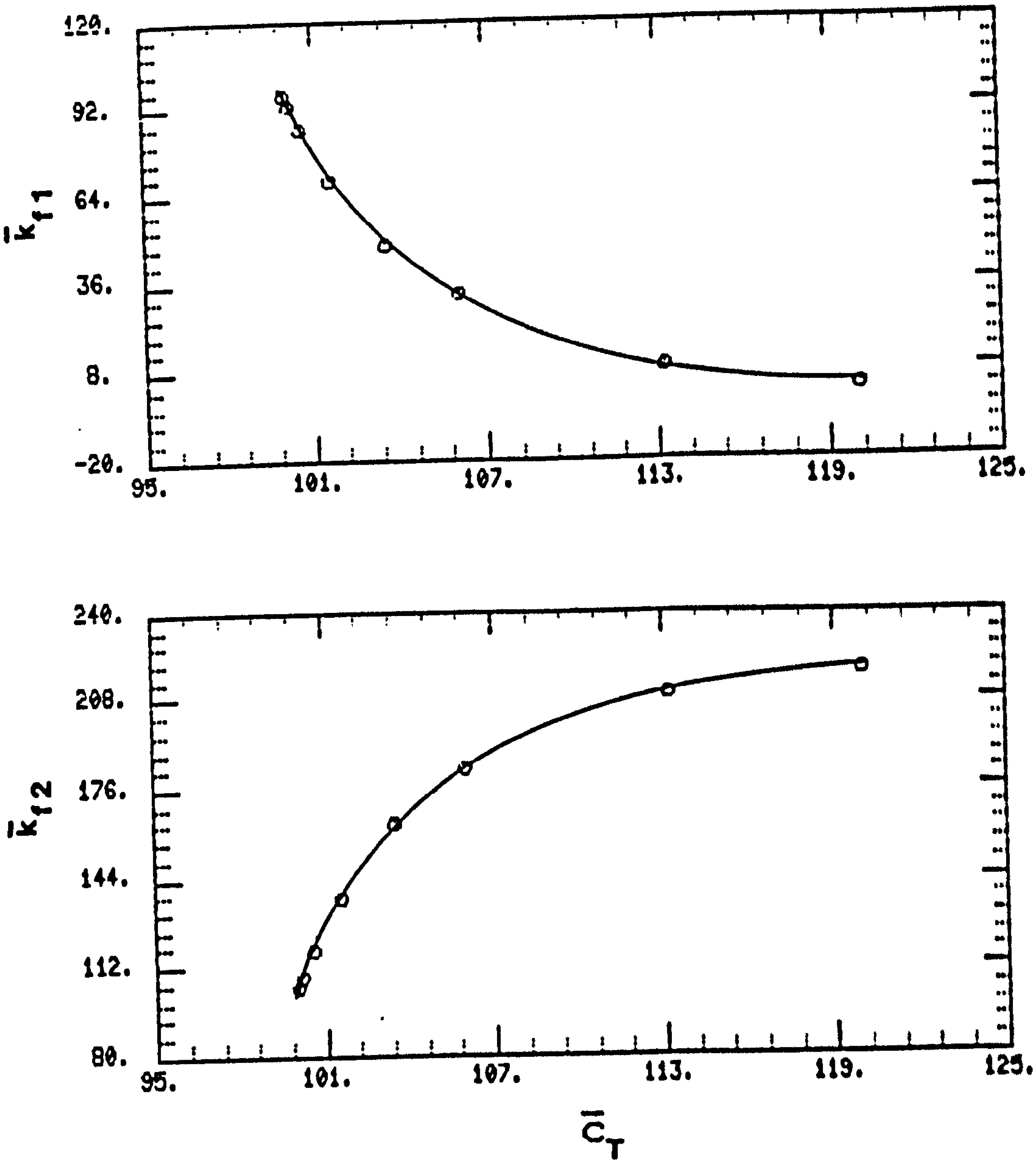

Figure 7.4 Secondary criteria

Table 7.5 Secondary criteria

Solution	$\bar{k}_{f1}$	$\bar{k}_{f2}$
S1	100.00	100.00
S2	91.40	110.14
S3	79.83	123.96
S4	73.85	132.31
S5	46.31	165.06
S6	32.98	182.62
S7	8.65	211.00
S8	2.07	219.01

In region I large reductions in the Bristol number can be obtained at the expense of small increases in the distillation column costs. If, for example, 0.55% increase in the total cost is accepted then a design whose BN is 32.4% smaller than that of the minimum costs design can be obtained. In most cases such a tradeoff is accepted and this region is eliminated from further consideration. In region III the total cost increases by an average of 2% for a mere 1% reduction in b_{11}. This expensive tradeoff coupled with the fact that the cost is already high suggest that this region can also be eliminated from further consideration. The remaining solutions from which the best design is to be chosen, are those belonging to region II. At this stage, the secondary and subjective criteria may have a large influence on the designer's decisions. The importance of the secondary criteria is highly dependent on the frequency at which changes in the distillation feed rate occur. Assume that solution S4 is chosen as the best design which is here referred to as design B. Its characteristics are given in table 7.6.

Table 7.6 Characteristics of design B

Design variables:	$R=5.5654$, $X_D=0.97593$, $X_B=0.00612$, $D=0.5093$, $B=0.4908$, $L=2.8342$, $V=3.3435$, $R_m=5.3911$, $N_m=30$, $N_T=85$, $N_F=47$.
Dynamic parameters and plant gains:	$L_R=12.1$, $T_s=3.299$, $T_1=3.231$, $T_2=0.358$, $T_3=0.100$, $T_4=0.098$, $T_z=-0.082$, $k_{11}=1.1916$, $k_{12}=-1.1298$, $k_{21}=0.7397$, $k_{22}=-0.8039$
Design criteria:	$C_T=0.24176$, $b_{11}=7.85$, $k_{f1}=0.4001$, $k_{f2}=0.5912$.

In design B, the Bristol number has been reduced by

45.9% at the expense of 1.58% increase in the total steady state cost. The steady state gain relating changes in the top product composition to changes in the feed rate is 26.2% smaller than its counterpart for design A whereas the gain relating variations in the feed rate has been increased by 32.3%. For design B the minimum condition number has a value of 29.3 which means it is 47.8% smaller than its counterpart value for design A.

7.6.4 Closed loop dynamic behaviour of designs A and B

The Wahl and Harriott transfer function matrices for designs A and B are as follows:

Design A:

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \dfrac{1.288}{3.81s+1} & \dfrac{-1.257}{3.81s+1} \\ \dfrac{0.6644}{3.81s+1} & \dfrac{-0.696}{3.81s+1} \end{bmatrix} \begin{bmatrix} \ell \\ v \end{bmatrix}$$

$$+ \begin{bmatrix} \dfrac{0.542(-0.070s+1)}{(3.81s+1)(0.34s+1)} \\ \dfrac{0.447}{3.81s+1} \end{bmatrix} f \qquad (7.78)$$

Design B:

$$\begin{bmatrix} x_D \\ \\ x_B \end{bmatrix} = \begin{bmatrix} \dfrac{1.192}{3.23s+1} & \dfrac{-1.130}{3.23s+1} \\ \dfrac{0.740}{3.23s+1} & \dfrac{-0.804}{3.23s+1} \end{bmatrix} \begin{bmatrix} \ell \\ \\ v \end{bmatrix}$$

$$+ \begin{bmatrix} \dfrac{0.400(-0.082s+1)}{(3.23s+1)(0.358s+1)} \\ \\ \dfrac{0.591}{3.23s+1} \end{bmatrix} f \qquad (7.79)$$

The complete control system is as shown in figure 7.1. The two plant controllers are Proportional plus Integral (PI) whose optimal parameters, which are given in table 7.7, have been determined using a two step approach. The multiloop sequential 1-2 method of Bhalodia and Weber [1979] was first used to obtain initial guesses for these best controllers settings followed by a trial and error optimization approach. The speed and oscillation of the time responses to a step change in the feed rate has been employed as the criteria for judging different sets of controllers parameters.

The optimal closed loop responses of designs A and B to a 1% step change in the load disturbance (feed rate) are shown in figures 7.5 and 7.6 respectively. Notice the sluggishness of design A responses which is due to the high interaction of the two loops. One might think that such slow responses can be speeded up by eliminating the interaction through the use of a decoupler. However, highly interactive systems with a large Bristol number are also highly sensitive to modeling errors. Such errors are always present in any real system and hence the inclusion of a decoupler may not improve on the performance of the interactive system for which it is designed or, indeed, it may even have a detrimental effect. Cases where the use of decouplers have led to unstabilisable systems have been reported by Weischedel [1981].

Table 7.7 Optimal controller parameters

Control loop	design A	design B
x_D--ℓ loop		
Proportional gain	17.0	20.0
Integral time	1.2	1.2
x_B--v loop		
Proportional gain	-30.0	-20.0
Integral time	1.0	1.0

Consider the following overall closed loop performance index:

$$\text{SITAE} = \int_0^{20} t\{(x_{Dset} - x_D)^2 + (x_{Bset} - x_B)^2\}dt \qquad (7.80)$$

where subscript (set) refers to set point.

For design A, SITAE, the Sum of the Integral of Time multiplied by the Absolute Error, has a value of 1.893 whereas that for design B has a value of 1.03. The superiority of the quality of control of design B (the best design) over that of the minimum costs design is quite apparent; the value of SITAE for design B is 45.6% smaller than its value for design A. The fact that the minimum condition number of design B is much smaller than that of design A indicates that the presence of modeling errors will result in a much more pronounced difference in the performance of the two designs.

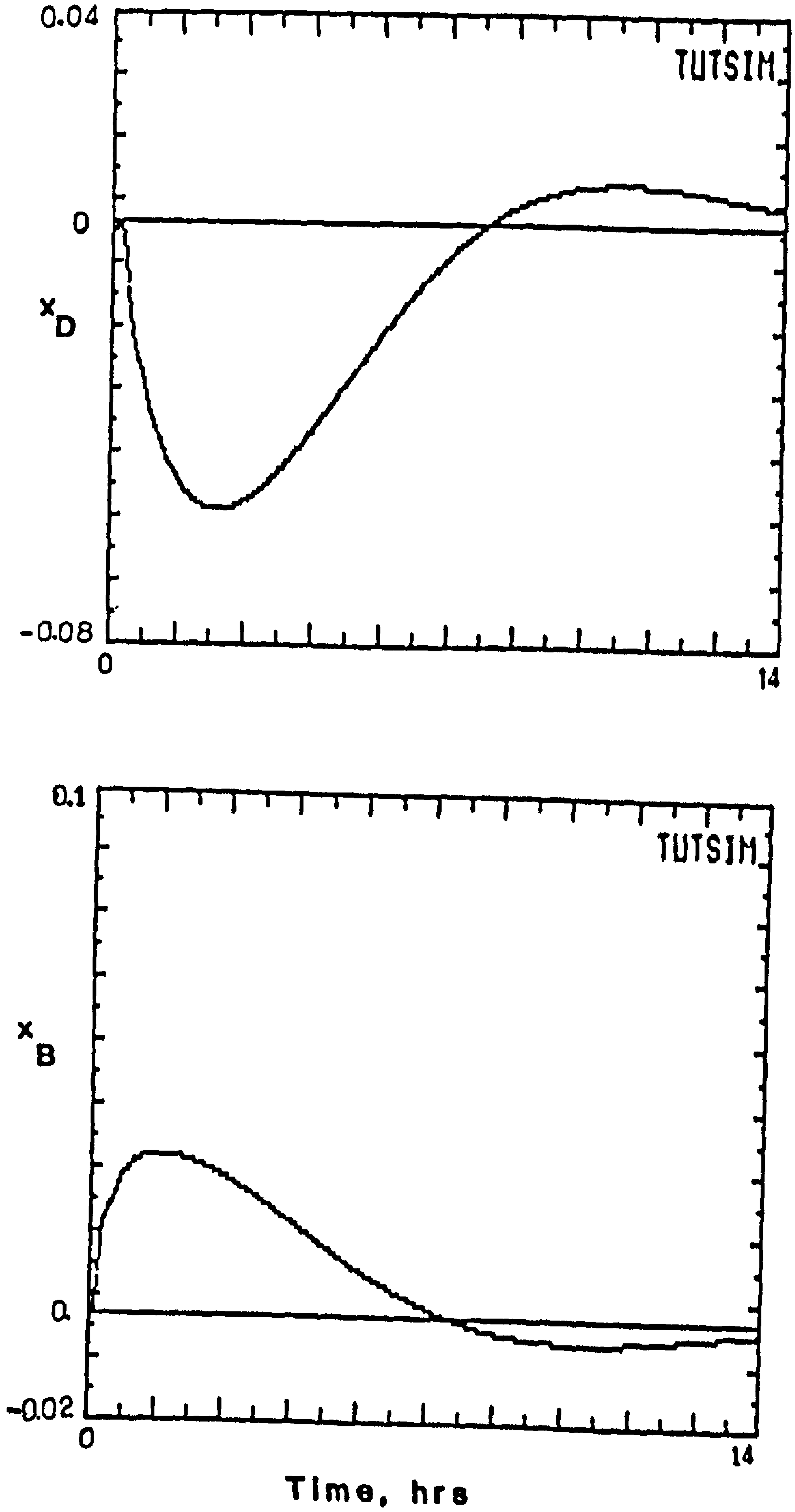

Figure 7.5 Closed loop responses of design A

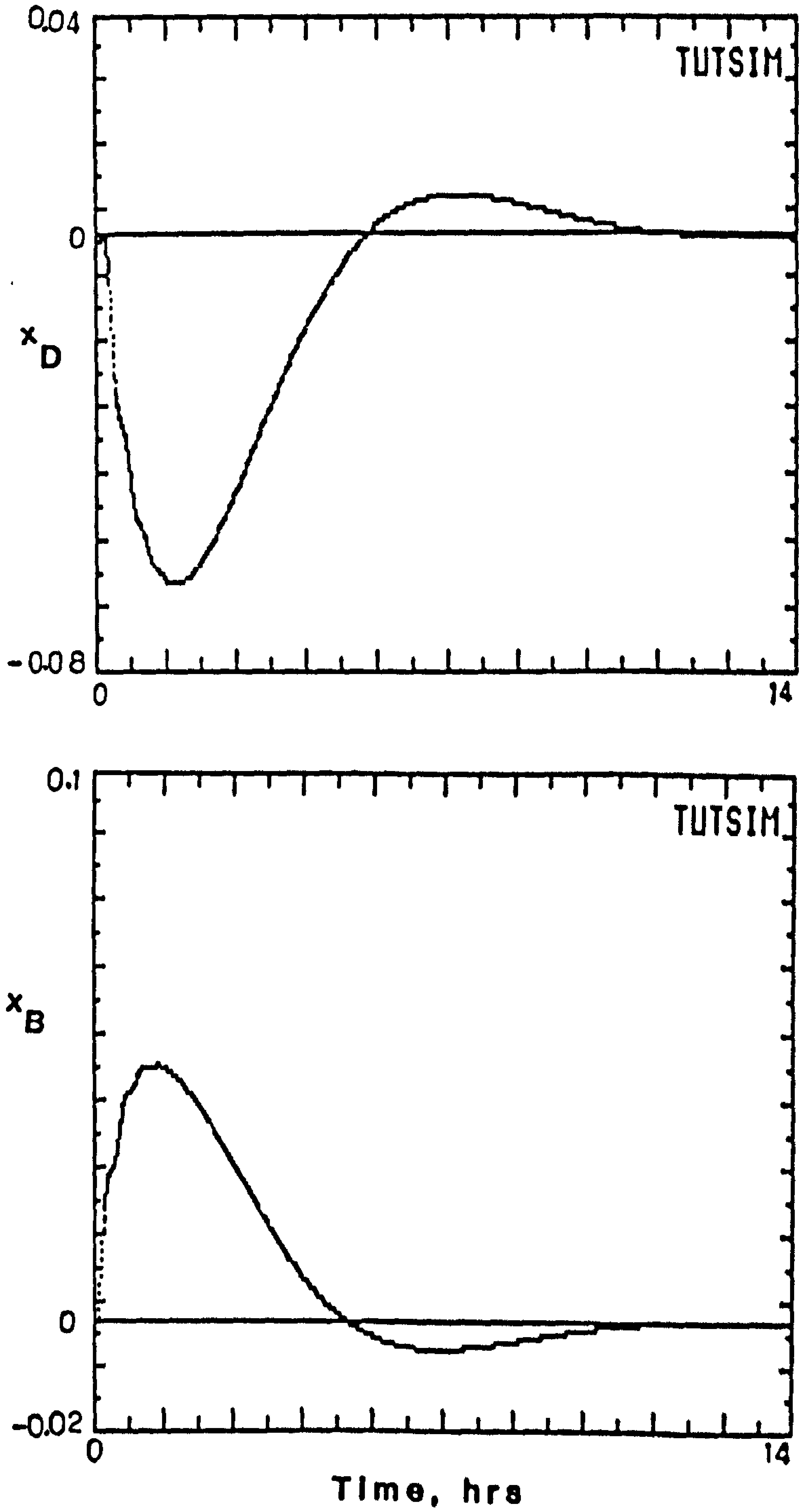

Figure 7.6 Closed loop responses of design B

APPENDIX 7A

ESTIMATION OF THE COST FACTORS

Table 7A.1 below gives the economic data needed for calculating the cost factors.

Table 7A.1 Economic data (1984)

Payout time = 2 years

Installed column cost = 1702 $/(m^2)(plate)

Average incremental cost of the condenser and reboiler = 302.5 $/(m^2)

Maintenance charges = 5%/year

Cost of steam = 1.934×10^{-3} \$/kg

Cost of cooling water = 2.784×10^{-5} \$/l

Total annual operating time = 8320 hr

Penalty for loosing isobutane in the bottom product, B_4=2.6652 \$/Kmole

Penalty for loosing n-butane in the top product, B_5=1.3282 \$/Kmole

Apart from the costs associated with products losses, all of the above data are based on those values given by Happel and Jordan [1975], pp. 388-91, which have been assumed to be 1975 costs. The Marshall and Swift Index, see Chemical Engineering (April 29, 1985, p.76), has been used to estimate their equivalent 1984 costs. The values of B_4 and

B_5 are those used by Shinskey [1984], p. 326.

Capital costs:

Column:

$$C_1 = 1702 \frac{\$}{m^2.\text{plate}}\left(\frac{1}{2\ \text{yr}} + \frac{0.05}{\text{yr}}\right)$$

$$C_1 = 936.1 \frac{\$}{m^2.\text{yr.plate}} \times \frac{\text{yr}}{8320\ \text{hr}}$$

$$C_1 = 0.113 \frac{\$}{m^2.\text{plate.hr}}$$

Using equation (7.44) we get:

$$B_1 = \frac{0.113 \dfrac{\$}{m^2.\text{plate.hr}} \times 58 \dfrac{\text{kg}}{\text{Kmole}}}{2196 \dfrac{m}{\text{hr}} \times 11.135 \dfrac{\text{kg}}{m^3}}$$

$$B_1 = 2.6804\text{x}10^{-4} \frac{\$}{\text{plate.Kmole}}$$

Reboiler and condenser

$$C_2 = 302.5 \frac{\$}{m^2}\left(\frac{1}{2\ \text{yr}} + \frac{0.05}{\text{yr}}\right)$$

$$C_2 = 166.4 \frac{\$}{m^2.yr} \times \frac{yr}{8320\ hr}$$

$$C_2 = 2x10^{-2} \frac{\$}{m^2.hr}$$

According to equation (7.50) we have:

$$B_2 = \frac{2x2x10^{-2} \frac{\$}{m^2.hr} \times 17523 \frac{Kj}{Kmole}}{2044 \frac{Kj}{hr.m^2.^\circ C}(16.5\ ^\circ C)}$$

$$B_2 = 2.06x10^{-2} \frac{\$}{Kmole}$$

Utilities costs:

Reboiler:

$$\text{Steam cost} = \frac{1.934x10^{-3} \frac{\$}{kg} \times 17523 \frac{Kj}{Kmole}}{2091 \frac{Kj}{kg}}$$

$$\text{Steam cost} = 1.6203x10^{-2} \frac{\$}{Kmole}$$

Condenser:

$$\text{Coolant cost} = \frac{2.784\times10^{-5}\ \frac{\$}{1} \times 17523\ \frac{\text{Kj}}{\text{Kmole}}}{4.19\ \frac{\text{Kj}}{1.^{\circ}\text{C}}\ (46\ ^{\circ}\text{C} - 26.5\ ^{\circ}\text{C})}$$

$$\text{Coolant cost} = 6.0\times10^{-3}\ \frac{\$}{\text{Kmole}}$$

The combined cost of vapourising and condensing 1 Kmole of vapour is:

$$B_3 = 1.6203\times10^{-2}\ \frac{\$}{\text{Kmole}} + 6.0\times10^{-3}\ \frac{\$}{\text{Kmole}}$$

$$B_3 = 2.2203\times10^{-2}\ \frac{\$}{\text{Kmole}}$$

APPENDIX 7B

Table II. Calculation of Plate Composition Gains*

Step 1. Determination of a_n and b_n

n	b_n	Common Term $= \xi$
0	1	0
1	$1/K_1$	0
$2, \ldots N_r$	$\left[\frac{VK_{n-1}+L}{VK_n}\right] b_{n-1} - \frac{L}{VK_n} b_{n-2}$	$\left[\frac{VK_{n-1}+L}{VK_n}\right] a_{n-1} - \frac{L}{VK_n} a_{n-2}$
N_r+1	$\left[\frac{VK_{n-1}+L_s}{VK_n}\right] b_{n-1} - \frac{L}{VK_n} b_{n-2}$	$\left[\frac{VK_{n-1}+L_s}{VK_n}\right] a_{n-1} - \frac{L}{VK_n} a_{n-2}$
$N_r+2, \ldots N_s$	$\left[\frac{VK_{n-1}+L_s}{VK_n}\right] b_{n-1} - \frac{L_s}{VK_n} b_{n-2}$	$\left[\frac{VK_{n-1}+L_s}{VK_n}\right] a_{n-1} - \frac{L_s}{VK_n} a_{n-2}$

	a_n for Load Shown				
n	Feed compn.	Feed rate	Reflux rate	Boilup rate	Equal reflux and boilup
0	0	0	0	0	0
1	0	0	0	0	0
$2, \ldots N_r$	0	0	$\xi + \frac{X_{n-1}-X_{n-2}}{VK_n}$	$\xi + \frac{Y_{n-1}-Y_n}{VK_n}$	$\xi + \frac{X_{n-1}-X_{n-2}}{VK_n} + \frac{Y_{n-1}-Y_n}{VK_n}$
N_r+1	$-\frac{F}{VK_n}$	$\xi + \frac{X_{n-1}-U}{VK_n}$	$\xi + \frac{X_{n-1}-X_{n-2}}{VK_n}$	$\xi + \frac{Y_{n-1}-Y_n}{VK_n}$	$\xi + \frac{X_{n-1}-X_{n-2}}{VK_n} + \frac{Y_{n-1}\ Y_n}{VK_n}$
$N_r+2, \ldots N_s$	ξ	$\xi + \frac{X_{n-1}-X_{n-2}}{VK_n}$	$\xi + \frac{X_{n-1}-X_{n-2}}{VK_n}$	$\xi + \frac{Y_{n-1}-Y_n}{VK_n}$	$\xi + \frac{X_{n-1}-X_{n-2}}{VK_n} + \frac{Y_{n-1}-Y_{n-2}}{VK_n}$

Step 2. Determination of condenser gain G_{ou}

For feed comp. load. $G_{ox} = \dfrac{F - Ba_R}{D + Bb_R}$

For feed rate load. $G_{oF} = \dfrac{X_f - X_R - Ba_R}{D + Bb_R}$

For reflux rate load. $G_{oL} = \dfrac{X_o - X_R - Ba_R}{D + Bb_R}$

For boilup rate load. $G_{oV} = \dfrac{X_R - X_o - Bb_R}{D + Bb_R}$

For equal reflux and boilup load. $G_{oV} = \dfrac{-Bb_R}{D + Bb_R}$

Step 3. Detetermination of gain on the plates
For all loads: $G_{nu} = a_n + b_n G_{ou}$ where a_n is the a_n for appropriate load u as given above

The approximate column time constant T_s is given as:

$$T_s = \frac{H_n G_{nu}}{BG_{Ru} + DG_{ou}}$$

* For the definition of the symbols used in this appendix see the paper of Wahl and Harriott (1970).

APPENDIX 7C

In this appendix, simple expressions for the steady state gains relating changes in the distillate and bottoms compositions to changes in the feed rate and composition are derived from Eduljee's [1975] equation. A procedure similar to that used by McAvoy [1983a], p. 121, is followed.

Eduljee's equation:

$$\frac{N - N_m}{N + 1} = 0.75\left[1 - \left(\frac{R - R_m}{R + 1}\right)^{0.5668}\right] \tag{7C.1}$$

where N is the total number of trays including the reboiler, i.e. $N = N_T - 1$

The following equations which have been given in section 7.2 are, for convenience, rewritten here as:

Overall material balance:

$$F = D + B \tag{7C.2}$$

Component material balance:

$$X_F F = X_D D + X_B B \tag{7C.3}$$

Minimum reflux ratio:

$$R_m = \frac{1}{\alpha-1}\left[\frac{X_D}{X_F} - \frac{\alpha(1-X_D)}{(1-X_F)}\right] \qquad (7C.4)$$

Minimum number of theoretical trays:

$$N_m = \frac{\ln\left[\frac{X_D(1-X_B)}{(1-X_D)X_B}\right]}{\ln(\alpha)} \qquad (7C.5)$$

7C.1 Feed rate load

The left hand side of equation (7C.1) is first differentiated with respect to F, holding the other column inputs (X_F, L, V) constant.

$$(LHS)' = \frac{-1}{N+1}(N_m)' \qquad (7C.6)$$

where the symbol ′ denotes the partial differentiation operator ∂/∂d. d is the load considered which is in this case F.

Differentiation of equation (7C.5) gives:

$$(N_m)' = \frac{1}{\ln(\alpha)}\left[\frac{1}{X_D(1-X_D)}(X_D)' - \frac{1}{X_B(1-X_B)}(X_B)'\right] \qquad (7C.7)$$

Substituting equation (7C.7) into equation (7C.6) gives:

$$(LHS)' = Z_1(X_D)' + Z_2(X_B)' \qquad (7C.8)$$

where,

$$Z_1 = \frac{-1}{X_D(1-X_D)(N+1)\ln(\alpha)} \qquad (7C.9)$$

$$Z_2 = \frac{1}{X_B(1-X_B)(N+1)\ln(\alpha)} \qquad (7C.10)$$

Differentiation of the right hand side of equation (7C.1) yields:

$$(RHS)' = 0.5668(0.75)\left(\frac{R-R_m}{R+1}\right)^{0.5668-1} \cdot \left(-\frac{1}{R+1}(R_m)'\right) \qquad (7C.11)$$

Using equation (7C.4) the following expression for $(R_m)'$ is obtained:

$$(R_m)' = \frac{1+X_F(\alpha-1)}{(\alpha-1)(1-X_F)X_F}(X_D)' \qquad (7C.12)$$

Equation (7C.1) can be rearranged as follows:

$$\left(\frac{R-R_m}{R+1}\right)^{0.5668} = 1 - \left(\frac{1}{0.75}\right)\left(\frac{N-N_m}{N+1}\right) \qquad (7C.13)$$

Combination of equations (7C.11) through (7C.13) yields:

$$(RHS)' = Z_4(X_D)' \qquad (7C.14)$$

where,

$$Z_4 = (-Z_3)\frac{(R+1)}{(R_m+1)}\left(\frac{\{(1+X_F(\alpha-1)\}}{(\alpha-1)(1-X_F)X_F}\right) \qquad (7C.15)$$

and

$$Z_3 = \frac{0.5668}{(R+1)(R-R_m)}\left[\frac{N-N_m}{N+1} - 0.75\right](R_m+1) \qquad (7C.16)$$

Equations (LHS)′ and (RHS)′, equations (7C.8) and (7C.14) respectively, to obtain:

$$(Z_1-Z_4)(X_D)' + Z_2(X_B)' = 0 \qquad (7C.17)$$

Combination of equations (7C.2) and (7C.3) gives the following relationship:

$$F(X_F-X_B) = D(X_D-X_B) \qquad (7C.18)$$

which is differentiated to yield:

$$(X_F-X_B) = D(X_D)' + F(X_B)' - D(X_B)' \tag{7C.19}$$

or

$$(X_F-X_B) = D(X_D)' + B(X_B)' \tag{7C.20}$$

The linear equations (7C.17) and (7C.20) are solved simultaneously to give expressions for the steady state gains $(X_D)'$ and $(X_B)'$ relating changes in the top and bottom products compositions, respectively, to changes in the feed rate.

$$(X_D)' = Z_2(X_B-X_F)/\{ B(Z_1-Z_4) - DZ_2 \} \tag{7C.21}$$

$$(X_B)' = \{ (X_F-X_B) - D(X_D)' \}/B \tag{7C.22}$$

7C.2 Feed composition loads

Following the same procedure, the gains relating changes in the condenser and reboiler compositions to upsets in the feed composition are obtained as:

$$(X_D)' = \frac{-(Z_5Z_7 + Z_2F/B)}{(Z_1 - Z_2D/B - Z_5Z_6)} \tag{7C.23}$$

$$(X_B)' = \{ F -D(X_D)' \}/B \tag{7C.24}$$

where,

$$Z_5 = -Z_3 \frac{(R+1)}{(R_m+1)} \cdot \frac{1}{(\alpha-1)} \tag{7C.25}$$

$$Z_6 = \{ 1/X_F + \alpha/(1-X_F) \} \tag{7C.26}$$

$$Z_7 = X_D/X_F^2 + \alpha(1-X_D)/(1-X_F)^2 \tag{7C.27}$$

CHAPTER 8

CONCLUSIONS AND RECOMMENDATIONS

In this investigation, a design approach which allows the simultaneous consideration of a number of criteria has been proposed. It is based on the field of Multiple Criteria Decision Analysis (MCDA).

In chapters 6 and 7, this algorithm has been applied to the integrated design and control of two unit operations, namely a CSTR and a binary n-butane--isobutane distillation column. In both cases it has been found that large improvements in the plant dynamic characteristics and degree of controllability can be achieved at the expense of small increases in the minimum total costs predicted by a steady state economic analysis. These two case studies clearly demonstrate the superiority of this newly proposed design algorithm over the currently practiced technique in which the controllability and operability aspects of the plant are seriously considered only after the plant design is completed. The suitability of this proposed multiobjective design approach can be enhanced through its application to the design of chemical plants consisting of a number of interconnected unit operations.

Since the design of process controllers is in itself a multiple criteria problem, in chapter 5 the proposed algorithm has been applied to the design of SISO controllers. Again, the superiority of this method over the currently practiced frequency and time domain techniques is clearly illustrated by the considered examples. Future work should consider the application of this design approach to the design of MIMO controller design problems.

Time delays, right half plane zeros, manipulated variables saturation and the plant sensitivity to modeling errors have been shown to be characteristics which prevent the achievement of perfect control and limit the quality of control obtained from practical control systems. Despite the recent attempts, reliable measures of the process degree of controllability and control difficulties presented to the control system are not available. Further research is needed which will hopefully lead to the development of generic, simple controllability measures to be used in the assessment of the operability and controllability of chemical processes. It appears, however, that any proposed measures should take into consideration the process controllers used as the deterioration of closed loop performance resulting from these limiting plant characteristics is dependent on the controllers employed.

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